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L2          841 SEA SSS FUL L1
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               E GALL M/AU
L8           46 SEA ABB=ON  PLU=ON  ("GALL M"/AU OR "GALL M A"/AU OR "GALL M
               B"/AU OR "GALL M J"/AU OR "GALL M P"/AU)
               E GALL MARTIN/AU
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               E BELL S/AU
L10         111 SEA ABB=ON  PLU=ON  ("BELL S"/AU OR "BELL S C"/AU)
               E BELL STAN/AU
L11         242 SEA ABB=ON  PLU=ON  ("BELL STAN"/AU OR "BELL STANELY C"/AU OR
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               CHARLES"/AU)

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L12           2 SEA ABB=ON  PLU=ON  L5
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               EDIT E1-E2 /AN /OREF

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L13           3 SEA ABB=ON  PLU=ON  ("CA54:4573G"/OREF OR "CA59:9970A"/OREF)
L14          20 SEA ABB=ON  PLU=ON  L6 OR L13
L15           0 SEA ABB=ON  PLU=ON  L14 AND (L7 OR L8 OR L9 OR L10 OR L11)
L16             QUE ABB=ON  PLU=ON  PY<=2000 OR AY<=2000 OR PRY<=2000
L17          19 SEA ABB=ON  PLU=ON  L14 AND L16

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FILE 'REGISTRY' ENTERED AT 08:35:19 ON 04 MAY 2005
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STRUCTURE FILE UPDATES:    3 MAY 2005  HIGHEST RN 849720-40-7
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*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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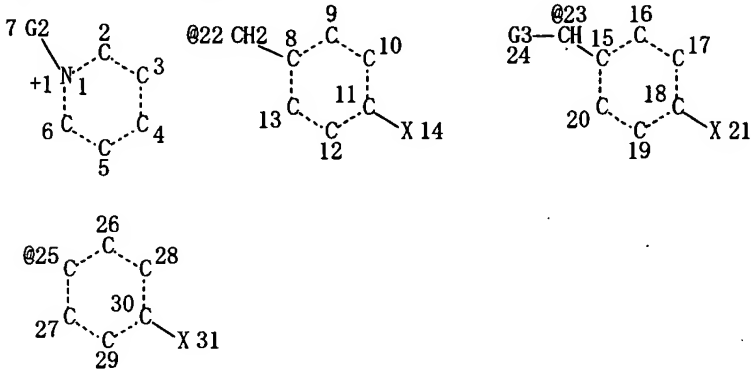

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DEFAULT ECLEVEL IS LIMITED

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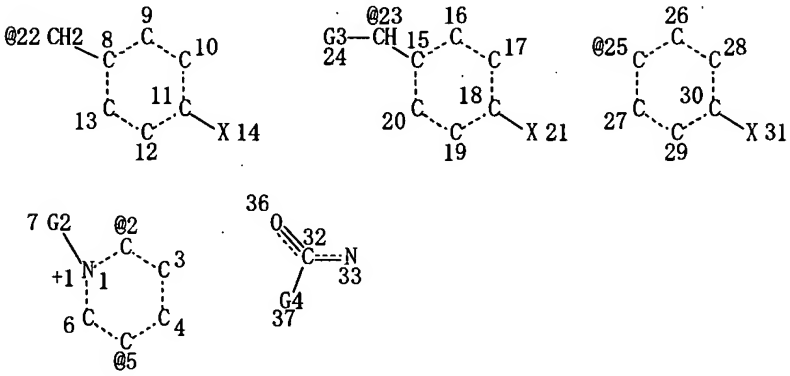
L3 STR



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DEFAULT MLEVEL IS ATOM
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE
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100.0% PROCESSED 46 ITERATIONS 46 ANSWERS
SEARCH TIME: 00.00.01

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FILE LAST UPDATED: 3 May 2005 (20050503/ED)

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=> d all hitstr l17 tot

L17 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:22735 HCAPLUS
DN 132:302951
ED Entered STN: 12 Jan 2000
TI ADP- and arachidonic acid (AA)-induced platelet aggregation inhibitory activity of carbamoylpyridines and carbamoylpiperidines
AU Youssef, Khairia M.; Al-Shafie, Faiza S.
CS Department of Medicinal Chemistry, College of Pharmacy, King Saud University, Riyadh, 11495, Saudi Arabia
SO Al-Azhar Bulletin of Science (**1998**), 9(2), 569-582
CODEN: ABSCE7; ISSN: 1110-2535
PB Al-Azhar University, Faculty of Science
DT Journal
LA English
CC 1-3 (Pharmacology)
AB N1-(3-pyridinylcarbonyl)-N4-2-pyrimidinylpiperazine (1) was synthesized to prepare a series of N1-(1-aralkyl or aroyl-3-pyridiniumylcarbonyl)-N4-2-pyrimidinyl piperazine halides (2a-g), which were then reduced to the corresponding N1-(1 -aralkyl- or aroyl-3 - piperidinylcarbonyl)-N4-Pyrimidinyl-piperazine hydrohalides (3a-g). Also, 1,4-bis (3 - pyridinylcartonyl) piperazine (4) and 1,4-bis(1-aralkyl-3 pyridiniumylcarbonyl) piperazine halides (5a,b) were prepared Thirteen compds. were tested for their inhibitory activity on ADP-and AA-induced aggregation of human platelets. As carbamoylpyridines and carbamoylpiperidines contain the carbamoyl group which is necessary for activity, it appears that lipophilicity is the determinant factor. The results show that activity of these compds. as platelet aggregation inhibitors go hand by hand with increased lipophilicity. N1-(3-pyridinylcarbonyl)-N4-2-pyrimidinyl-piperazine (1), elicits high inhibitory activity on ADP- and AA-induced aggregations of human platelets which indicates that the structure possesses the pharmacophore responsible for inhibition i.e. the carbamoyl group attached to the lipophilic cycloalkyl groups. N1 -(1 -p-Aminobenzyl-3 -piperidinylcarbonyl)-N4-2-

pyrimidinyl-piperazine (3b) is the most active compound which shows total inhibition for both ADP- and AA-induced aggregation of human platelets. 1,4-Bis (3-pyridinyl-carbonyl) piperazine (4), shows both primary phase inhibition for the ADP-induced aggregation and total inhibition for AA-induced aggregation. On the other hand, 1,4-Bis (1-aralkyl-pyridinium-3-ylcarbonyl) piperazine halides (5a,b) shows no activity, most probably, because of the high polarity resulted from the dicationic character.

ST carbamoylpyridine carbamoylpiperidine deriv prepn structure platelet aggregation inhibitor

IT Pharmacophores
(carbamoyl group attached to lipophilic cycloalkyl groups; carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT Lipophilicity
Platelet aggregation inhibitors
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT Structure-activity relationship
(platelet aggregation-inhibiting; carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT 17433-19-1P 160539-75-3P 265123-01-1P 265123-02-2P 265123-03-3P **265123-04-4P** 265123-05-5P **265123-06-6P** 265123-07-7P 265123-08-8P 265123-14-6P **265123-15-7P** **265123-16-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT 58-64-0, Adp, biological studies 506-32-1, Arachidonic acid
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT 59-67-6, Nicotinic acid, reactions 110-85-0, Piperazine, reactions 110-86-1, Pyridine, reactions 20980-22-7, 1-(2-Pyrimidinyl)piperazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT 10400-19-8P, Nicotinic acid chloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

IT 265123-09-9P 265123-10-2P 265123-11-3P 265123-12-4P 265123-13-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

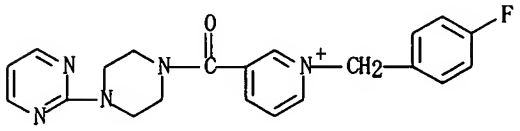
(1) Chap, H; Agents Actions 1979, V9, P400406
(2) Edmunds, L; Ann Thorac Surg 1987, V44, P430
(3) Feng, Z; J Med Chem 1992, V35, P2952 HCAPLUS
(4) Fuster, V; Circulation 1982, V66(Suppl 1), P157
(5) Gollamudi, R; Biochem Biophys Res Commun 1991, V177, P888 HCAPLUS
(6) Harker, L; J Am Coll Cardiol 1986, V8, P21B HCAPLUS
(7) Harker, L; Thromb Hemastasis 1986, V12, P134 MEDLINE
(8) Lam, J; Deposition and Mural Thrombosis J Am Colt Cardiol 1986, V8, P1380 MEDLINE
(9) Lasslo, A; Am Soc Art Int Organs 1983, V6, P47 HCAPLUS
(10) Lasslo, A; J Org Chem 1957, V22, P837 HCAPLUS
(11) Lasslo, A; Med Prog Technol 1986, V11, P109 MEDLINE
(12) Lasslo, A; Res Commun Chem Path Pharmacol 1990, V69, P133 HCAPLUS
(13) Nozawa, Y; Biochim Biophys Acta 1991, V1082, P219 HCAPLUS
(14) Quintana, R; J Pharm Sci 1963, V52, P1186 MEDLINE
(15) Quintana, R; J Pharm Sci 1965, V54, P735
(16) Quintana, R; Thromb Res 1980, V20, P405 HCAPLUS
(17) Quintana, R; Thromb Res 1981, V24, P379 HCAPLUS
(18) Quintana, R; Thromb Res 1981, V22, P665 HCAPLUS
(19) Shattil, S; Biochemistry 1976, V15, P4832 HCAPLUS

Search done by Noble Jarrell

(20) Shephard, L; Trends Biotech 1991, V9, P80
(21) Solymoss, B; Circulation 1988, V78(Suppl 1), P140
(22) Stein, B; J Am Coll Cardiol 1989, V14, P813 HCAPLUS
(23) Tucker, T; J Med Chem 1997, V40, P830 HCAPLUS
(24) Webster, M; Platelets in Health and disease 1990, P265 MEDLINE

IT **265123-04-4P 265123-06-6P 265123-15-7P**
265123-16-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(carbamoylpyridines and carbamoylpiperidines inhibition of ADP- and arachidonic acid-induced platelet aggregation)

RN 265123-04-4 HCAPLUS
CN Pyridinium, 1-[(4-fluorophenyl)methyl]-3-[[4-(2-pyrimidinyl)-1-piperazinyl]carbonyl]-, chloride (9CI) (CA INDEX NAME)



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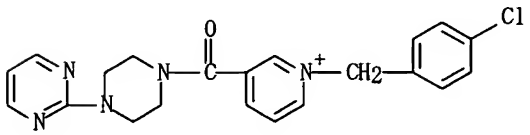
RN 265123-06-6 HCAPLUS
CN Pyridinium, 1-[(4-chlorophenyl)methyl]-3-[[4-(2-pyrimidinyl)-1-piperazinyl]carbonyl]-, chloride (9CI) (CA INDEX NAME)



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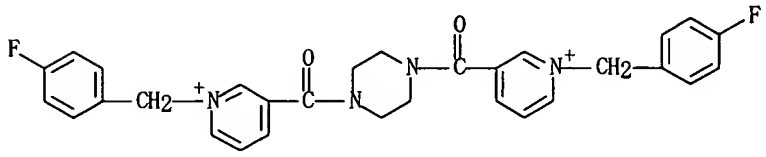
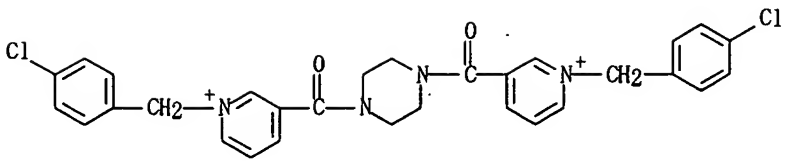
RN 265123-15-7 HCAPLUS
CN Pyridinium, 3,3'-(1,4-piperazinediyldicarbonyl)bis[1-[(4-fluorophenyl)methyl]-, dichloride (9CI) (CA INDEX NAME)



●2 Cl^-

RN 265123-16-8 HCAPLUS
CN Pyridinium, 3,3'-(1,4-piperazinediyldicarbonyl)bis[1-[(4-chlorophenyl)methyl]-, dichloride (9CI) (CA INDEX NAME)



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L17 ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:619241 HCAPLUS
DN 125:300276
ED Entered STN: 18 Oct 1996
TI Reactions of Charged Substrates. 5. The Solvolysis and Sodium Azide Substitution Reactions of Benzylpyridinium Ions in Deuterium Oxide
AU Buckley, Neil; Oppenheimer, Norman J.
CS Department of Pharmaceutical Chemistry, University of California, San Francisco, CA, 94143-0446, USA
SO Journal of Organic Chemistry (**1996**), 61(21), 7360-7372
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 7
AB Second-order rate consts. and activation values were measured for the reactions with NaN3 of a series of 4-Y-substituted (Y = MeO, Me, H, Cl, and NO2) benzyl 3'-Z-substituted (Z = CN, CONH2, H, F, Ac) pyridinium chlorides in deuterium oxide. 3'-Cyanopyridine substrates reacted much faster than nicotinamide and pyridine substrates; in the pyridine series the 4-Me, 4-H, and 4-Cl benzyl analogs did not react for up to 6 mo at 96° in 1.7 M NaN3. The 3'-cyanopyridine substrates do not exhibit borderline kinetic behavior, but the nicotinamide substrates do. The Hammett plot is flat for the NaN3 reaction of 3'-cyanopyridine substrates and increasingly V-shaped for the nicotinamide and pyridine substrates. The values of βLG (four-point plot) for the NaN3 reaction of the 4-MeO benzyl substrates is -1.45, which is usually interpreted as being a very "late" activated complex. Two-point Bronsted "plots" for the other benzyl derivs. and for two N-methylpyridinium ions give values of βLG in the same range. The second-order rate constant and activation values for N-methyl-3'-cyanopyridinium iodide are within the same range as those for the benzyl substrates. For the hydrolysis reaction, the Hammett plot is linear for 3'-cyanopyridine substrates (ρ^+ = -1.24) and flat for the nicotinamide substrates. The extent of hydrolysis of 0.005-0.05 M solns. of the 3'-cyanopyridinie substrates depended on the initial concentration of substrate, and hydrolysis was slowed significantly or stopped completely in the presence of exogenous 3-cyanopyridine. These results show that an equilibrium is established among the products for the 4-MeO, 4-Me, 4-H, and 4-Cl substrates; the 4-NO2 substrate reacted too slowly to discern any difference. Data for the extent of hydrolysis were fitted by an equation derived assuming the equilibrium Despite this limitation on a classic test of mechanism, the rates and ρ values are consistent with direct displacement by solvent and not with a unimol. process. These results, which are rationalized in terms of the Pross-Shaik model, suggest that there are no ion-dipole complex intermediates in the benzyl series and show that borderline kinetic behavior is a function of leaving group ability and is not necessarily related to a change in mechanism. A computational approach was used to evaluate anomalous βLG values for the hydrolysis and nucleophilic substitution reactions of the methylpyridinium ion substrates. It was found that neither the Nu-substrate bond lengths nor the difference in charge matched the βLG values. The value of ΔΔS. thermod. of -15 gibbs/mol between (4-methoxybenzyl)-3'-cyanopyridinium chloride and the corresponding dimethylsulfonium chloride in the NaN3 reaction, which is the result of the solvation of the pyridine at the transition state and

the lack of solvation of SMe2, is used to argue that the source of NAD+ glycohydrolase "catalysis" of NAD+ bond cleavage is the result of desolvation of the leaving group upon binding.

ST benzylpyridinium hydrolysis azide substitution kinetics mechanism; reaction const benzylpyridinium hydrolysis azide substitution; NAD glycohydrolase catalysis

IT Electron configuration and Electron density
Heat of hydrolysis
Hydrolysis
Kinetics of hydrolysis
Leaving group effects
Linear free energy relationship
Potential energy surface and hypersurface
Reaction constant
Substituent effect
Substitution reaction, nucleophilic
Transition state structure
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Pyridinium compounds
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Molecular orbital
(frontier, kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Heat of substitution reaction
Kinetics of substitution reaction
(nucleophilic, kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT 2876-13-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(estimated; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

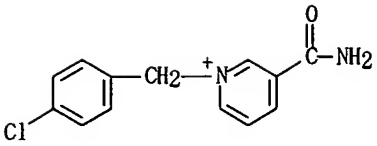
IT 594-09-2, Trimethylphosphine 1004-16-6, 3-Cyano-1-methylpyridinium iodide 4329-72-0 5096-13-9 6456-44-6 6621-73-4 **6951-52-6** 14343-69-2, Azide 14535-08-1 14535-12-7 20461-54-5, Iodide, reactions 26628-22-8, Sodium azide 52354-19-5 63828-55-7 74796-72-8 76053-06-0 87976-56-5 98349-72-5 183054-49-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT 7732-18-5, Water, reactions 15923-33-8 183054-50-4
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(potential surface calcn.; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT **6951-52-6**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

RN 6951-52-6 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



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L17 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:191937 HCAPLUS
DN 124:316412
ED Entered STN: 04 Apr 1996
TI Reactions of Charged Substrates. 4. The Gas-Phase Dissociation of (4-Substituted benzyl)dimethylsulfoniums and -pyridiniums
AU Buckley, Neil; Maltby, David; Burlingame, Alma L.; Oppenheimer, Norman J.
CS School of Pharmacy, University of California, San Francisco, CA, 94143-0446, USA
SO Journal of Organic Chemistry (**1996**), 61(8), 2753-62
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-12 (Physical Organic Chemistry)
Section cross-reference(s): 33
AB The relative rates for the gas-phase dissociation RX+ → R+ + X° of five (4-Y-substituted benzyl)dimethysulfoniums (Y = MeO, Me, H, Cl, and NO2) and 24 (4-Y-substituted benzyl)-3'-Z-pyridiniums (complete series for Z = CN, Cl, CONH2, and H, and 4-methoxy- and 4-nitrobenzyls for Z = F and CH3CO) were measured using liquid secondary ion mass spectrometry. The Hammett plot (vs δΔG0 or σ+) is linear for the sulfoniums, but plots for the four pyridinium series have a drastic break between the 4-Cl and 4-NO2 substrates. Broensted-like plots for the pyridiniums show a strong leaving group effect only for 4-nitrobenzyls. An anal. of these linear free energy relations with supporting evidence from semiempirical computations suggests that collisionally activated pyridinium substrates dissociate through two pathways, direct dissociation and an ion-neutral complex intermediate. Comparison of these results with results for the solution reactions of some of these compds. shows that the mechanism is different in the gas and solution phases. Sufficient exptl. data are not available to assign a mechanism for dissociation to the sulfonium series, but computational results show characteristics of a direct dissociative mechanism.
ST dissocn gas phase benzyldimethylsulfonium benzyldimethylpyridinium; sulfonium benzyldimethyl gas phase dissocn; pyridinium benzyldimethyl gas phase dissocn
IT Linear free energy relationship
Reaction constant
(for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)
IT Dissociation
Kinetics of dissociation
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)
IT Leaving group effects
Substituent effect
(on gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)
IT Linear free energy relationship
(Broensted, for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)
IT 15519-25-2 16183-83-8 16183-87-2 24837-70-5 38332-27-3
45809-04-9 45964-81-6 46122-80-9 46441-13-8 48120-95-2
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133227-04-0 175979-55-2 **175979-56-3** 175979-57-4

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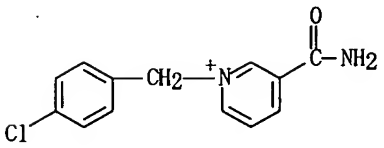
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT **175979-56-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

RN 175979-56-3 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]- (9CI) (CA INDEX NAME)

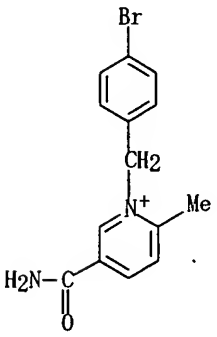


L17 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:422794 HCAPLUS
DN 113:22794
ED Entered STN: 21 Jul 1990
TI Addition of cyanide ion to nicotinamide cations in acetonitrile. Formation of nonproductive charge-transfer complexes
AU Engbersen, Johan F. J.; Koudijs, Arie; Sleiderink, Hedwig M.; Franssen, Maurice C. R.
CS Lab. Org. Chem., Agric. Univ., Wageningen, 6703 HB, Neth.
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (**1990**), (1), 79-83
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
OS CASREACT 113:22794
AB The mixing of equal vols. of 0.2 mmol dm-3 1-benzylnicotinamide ion and 2 mmol dm-3 cyanide ion results in the immediate formation of a transient absorption band at 375 nm which can be ascribed to a charge-transfer complex. This complex disappears within ca. 0.2 s with the formation of the 1,6-addition product which, in turn, is rapidly converted into the thermodynamically more stable 1,4-adduct. Me substitution at the 6-position of the nicotinamide ring inhibits the formation of the 1,6-adduct, resulting in an increase in the lifetime of the charge-transfer complex. Subsequently a mixture of the 1,4-cyanide adduct and, most likely, the 1,2-adduct is formed. Rate effects with variation of substituents in the 1-benzyl group reveal that charge-transfer complex formation is counterproductive to the formation of addition products.
ST cyanide ion addn nicotinamide cation; charge transfer complex cyanide nicotinamide; substituent effect cyanide addn nicotinamide
IT Reaction constant
(for addition, dissociation, and charge-transfer-complexation processes in cyanide ion-nicotinamide cation systems)
IT Addition reaction
(of cyanide ion with nicotinamide cations, formation of nonproductive charge-transfer complexes in)
IT Kinetics of addition reaction
(of cyanide ion with nicotinamide cations, solvent and substituent effects on)
IT Kinetics of dissociation
(of cyanide-ion adducts with nicotinamide cations, solvent and substituent effects on)
IT Ultraviolet and visible spectra
(of transient species, in addition reaction of cyanide ion with nicotinamide cations)

IT Substituent effect
(on addition, dissociation, and charge-transfer-complexation processes in cyanide ion-nicotinamide cation systems)
IT 151-50-8, Potassium cyanide (K(CN))
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with nicotinamide cations)
IT 127678-22-2 127678-24-4 127678-25-5 **127678-27-7**
127678-29-9
RL: PROC (Process)
(decay of, kinetics of)
IT 13076-43-2P **54027-58-6P** 63761-90-0P 63761-95-5P
63828-55-7P 70293-11-7P **127663-01-8P** 127663-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with cyanide)
IT 96551-72-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation and addition reaction of, with cyanide)
IT 127663-05-2P 127663-06-3P 127663-07-4P **127678-20-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation of, with cyanide)
IT 19432-61-2P 75420-69-8P 75420-70-1P 75420-71-2P 75420-74-5P
127663-03-0P 127663-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation of, kinetics of)
IT 127663-08-5P 127663-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **127678-27-7**
RL: PROC (Process)
(decay of, kinetics of)
RN 127678-27-7 HCAPLUS
CN Pyridinium, 5-(aminocarbonyl)-1-[(4-bromophenyl)methyl]-2-methyl-, cyanide (9CI) (CA INDEX NAME)

CM 1

CRN 127678-26-6
CMF C14 H14 Br N2 O

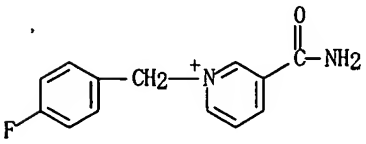


CM 2

CRN 57-12-5
CMF C N

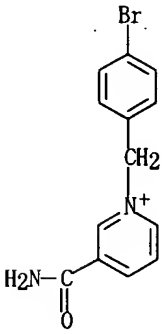
IT **54027-58-6P 127663-01-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and addition reaction of, with cyanide)
RN 54027-58-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, bromide (9CI)
(CA INDEX NAME)



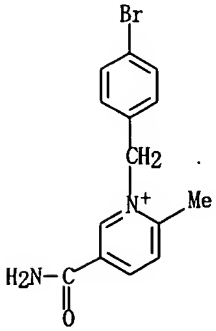
● Br^-

RN 127663-01-8 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-bromophenyl)methyl]-, bromide (9CI)
(CA INDEX NAME)



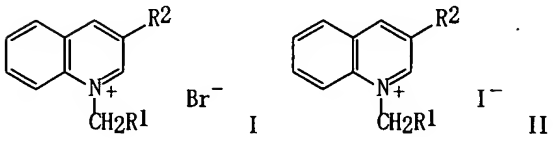
● Br^-

IT **127678-20-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation of, with cyanide)
RN 127678-20-0 HCAPLUS
CN Pyridinium, 5-(aminocarbonyl)-1-[(4-bromophenyl)methyl]-2-methyl-, bromide (9CI) (CA INDEX NAME)

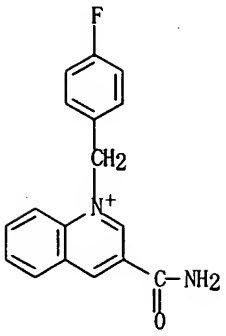


● Br^-

L17 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:610868 HCAPLUS
DN 109:210868
ED Entered STN: 10 Dec 1988
TI Iodide salts of nitrogen heterocycles by bromide-iodide exchange
AU Lee, In Sook Han; Lee, Chang Kiu; Han, In Sup
CS Dep. Sci. Educ., Kangweon Natl. Univ., Chuncheon, 200, S. Korea
SO Organic Preparations and Procedures International (**1988**), 20(3), 302-5
CODEN: OPPIAK; ISSN: 0030-4948
DT Journal
LA English
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 109:210868
GI

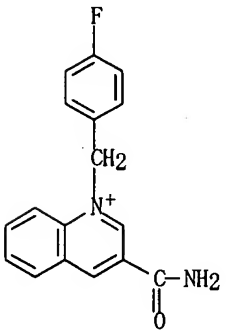


AB Quinolinium bromides I (R1 = Ph, tolyl, halophenyl, F3CC6H4; R2 = cyano, CONH2, H) were treated with KI in EtOH-water to give iodides II in good yields. Similarly prepared was 1-benzylpyridinium iodide.
ST quinolinium iodide benzyl; benzylquinolinium iodide; exchange iodide benzylquinolinium bromide
IT Exchange reaction
(bromide-iodide, of benzylquinolinium bromides with potassium iodide)
IT 7681-11-0, Potassium iodide, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, with benzylquinolinium bromides)
IT 2589-31-3, 1-Benzylpyridinium bromide 13076-43-2 26323-01-3 65674-20-6 70083-49-7 70293-11-7 87861-96-9 111977-04-9 111977-05-0 111977-06-1 111977-07-2 111977-08-3 111997-43-4 **117483-02-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, with potassium iodide)
IT 17260-82-1P 34931-23-2P 46210-32-6P 72306-81-1P 109653-23-8P 117483-03-1P 117483-04-2P 117483-05-3P 117483-06-4P 117483-07-5P 117483-08-6P 117483-09-7P 117483-10-0P **117483-11-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **117483-02-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, with potassium iodide)
RN 117483-02-0 HCAPLUS
CN Quinolinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

IT **117483-11-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 117483-11-1 HCAPLUS
CN Quinolinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, iodide (9CI)
(CA INDEX NAME)



● I^-

L17 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:166806 HCAPLUS
DN 108:166806
ED Entered STN: 13 May 1988
TI Polarographic reduction of p-substituted 1-phenyl-3-(aminocarbonyl)pyridinium salts
AU Krechl, Jiri; Mizaninoiva, Daniela; Volke, Jiri; Kuthan, Josef
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28, Czech.
SO Collection of Czechoslovak Chemical Communications (**1987**), 52(6), 1550-60
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 72
AB The substituent effect (H, NO2, CO2H, Br, Cl, NHAc, Me, OMe, OH, NEt2) on the polarog. behavior of p-substituted 1-phenyl-3-aminocarbonylpyridinium cations has been investigated, in particular on their half-wave potentials in aqueous phosphate buffers pH 6·65 (10% DMF) and in anhydrous solns. of DMF with 0·05 mol L-1 Bu4N+ BF4- as supporting electrolyte. The half-wave potentials of the reduction wave which corresponds to the uptake of a single electron (wave B) and to the formation of the primary radical,

obey a Hammett correlation in a way similar to the case of 1-benzyl-3-aminocarbonylpyridinium cations. The slope $Q\pi,R$ in the Hammett plot equals 0·093 V for 10% DMF and 0·179 V for anhydrous DMF and compares thus with the slope obtained with the 1-benzyl derivs. where 0.05 V was found for water and 0·127 V of anhydrous acetonitrile. The transfer of the substituent effect from the substituent in the para position on the benzene nucleus to the heterocyclic ring is thus equally active in both substances and depends more strongly on the solvent than on the structure of the cation of both types. The low sensitivity in both series towards a change in the substituent is explained by the fact that during the uptake of the electron the benzene and the pyridine nucleus are not even approx. coplanar. This is why the π-overlap between the two nuclei is considerably restricted. The anal. of sampled d.c.-polarog. waves has confirmed that the one-electron uptake is followed by a chemical reaction, most probably a dimer formation or a reaction of the primary product with the starting substance.

ST polarog redn pyridinium salt; amidopyridinium phenyl electrochem redn LFER

IT Reduction
(of substituted phenyl(aminocarbonyl)pyridinium salts, substituent effects on)

IT Substituent effect
(on polarog. reduction of phenyl(aminocarbonyl)pyridinium salts)

IT 5096-13-9 **6951-52-6** 52354-19-5 63828-55-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)

IT 54027-59-7P 54027-60-0P 69986-64-7P 76911-53-0P 76911-55-2P 76911-56-3P 87384-49-4P 87384-51-8P 87384-52-9P 112445-86-0P 113849-47-1P 113849-48-2P 113849-49-3P 113849-50-6P 113849-53-9P 113849-54-0P 113849-55-1P 113849-57-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and polarog. reduction of)

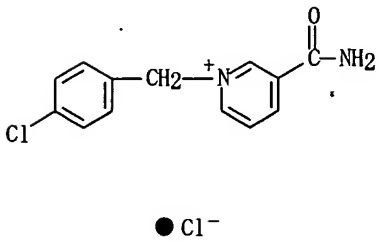
IT 98-92-0, Nicotinamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with anilines)

IT 62-53-3, reactions 93-05-0 100-01-6, reactions 104-94-9, 4-Methoxyaniline 106-40-1, 4-Bromoaniline 106-47-8, 4-Chloroaniline, reactions 106-49-0, reactions 122-80-5, 4-Acetamidoaniline 123-30-8, 4-Hydroxyaniline 150-13-0, 4-Aminobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nicotinamide)

IT **6951-52-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)

RN 6951-52-6 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L17 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:55309 HCAPLUS

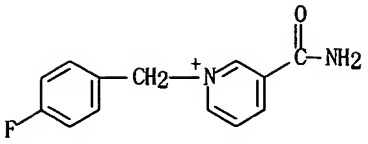
DN 108:55309

ED Entered STN: 20 Feb 1988

TI Structure sensitivity of the Marcus λ for hydride transfer between NAD+ analogs

AU Kreevoy, Maurice M.; Ostovic, Drazen; Lee, In Sook Han; Binder, David A.; King, Gary W.

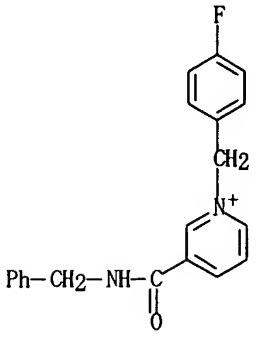
CS Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA
SO Journal of the American Chemical Society (**1988**), 110(2), 524-30
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 22-7 (Physical Organic Chemistry)
AB Thirty-five rate consts., kij, for transfer of hydride between various pyridinium, quinolinium, acridinium, and phenanthridinium ions spanning a range of over 1011 in their equilibrium consts. Kij and over 106 in kij have been measured. (All these ions can be regarded as analogs of NAD+.). Calcn. of these kij by conventional Marcus theory, with a constant, averaged value of the intrinsic barrier, λ, gives a fair level of agreement, with an average discrepancy of 0.9 between calculated and observed values of lin kij. Use of a structure-sensitive λ reduces this discrepancy to 0.5.
ST Marcus LFER hydride transfer; NADH analog hydride transfer
IT Kinetics of hydride transfer
(between NAD+ analogs)
IT Hydride transfer
(between NAD+ analogs, equilibrium consts. for)
IT Transition state structure
(for hydride transfer between NAD+ analogs)
IT Substituent effect
(on hydride transfer between NAD+ analogs)
IT Linear free energy relationship
(Broensted, for hydride transfer between NAD+ analogs)
IT Linear free energy relationship
(Marcus, for hydride transfer between NAD+ analogs)
IT 948-43-6 5412-06-6 6516-41-2 6516-53-6 13076-43-2 26368-94-5
50741-48-5 64433-61-0 70083-49-7 70293-11-7 98576-69-3
111977-04-9 111977-05-0 111977-06-1 111977-07-2 111977-08-3
111997-43-4
RL: PRP (Properties)
(hydride transfer between NAD+ analogs and, Marcus theory and equilibrium and kinetics for)
IT 92-81-9 952-92-1 3337-17-5 4217-54-3 5496-66-2 17260-79-6
19350-64-2 20224-92-4 27799-79-7 30319-92-7 37589-77-8
50624-35-6 **54027-58-6** 54732-80-8 57355-62-1 66875-56-7
72594-76-4 73184-18-6 87861-94-7 87861-95-8 87861-99-2
98576-64-8 98576-65-9 98576-66-0 98576-67-1 98576-70-6
111977-09-4 111977-10-7 111977-11-8 111977-12-9 111977-13-0
111977-14-1
RL: PRP (Properties)
(hydride transfer between, and NAD+ analogs, Marcus theory and equilibrium and kinetics for)
IT 53-84-9D, NAD+, analogs
RL: PRP (Properties)
(hydride transfer between, structure sensitivity of Marcus λ for hydride transfer)
IT 1333-74-0 12184-88-2
RL: PRP (Properties)
(hydride transfer, between NAD+ analogs, equilibrium consts. for)
IT 16969-45-2P 22559-70-2P 22559-71-3P 23686-76-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **54027-58-6**
RL: PRP (Properties)
(hydride transfer between, and NAD+ analogs, Marcus theory and equilibrium and kinetics for)
RN 54027-58-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, bromide (9CI) (CA INDEX NAME)



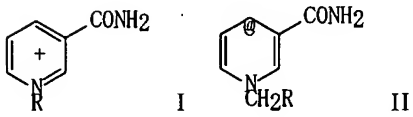
● Br^-

L17 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:575027 HCAPLUS
DN 99:175027
ED Entered STN: 12 May 1984
TI Hydride transfer between NAD+ analogs
AU Roberts, R. M. G.; Ostovic, D.; Kreevoy, M. M.
CS Dep. Chem., Univ. Minnesota, Minneapolis, MN, 55455, USA
SO Faraday Discussions of the Chemical Society (**1982**), (74), 257-65
CODEN: FDCSB7; ISSN: 0301-7249
DT Journal
LA English
CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 27
AB Rate (k) and equilibrium consts. (K) were measured for 17 nondegenerate hydride-transfer reactions, the donors and acceptors generally being variously substituted pyridinium ions. Rate consts. were also measured for 6 degenerate reactions of the same type. These results were used to test the Marcus theory of atom transfer. The Broensted plot shows a good deal of scatter, but around K = 1.0 it has about the predicted slope (α) of 0.5. Using the measured values of k for degenerate reactions and assuming reactivity to be constant within structural families, values of k for 12 nondegenerate reactions were calculated without introducing adjustable parameters. They reproduce 99% of the variation in the measured values, the latter generally exceeding the calculated values. The data do not permit a test of the predicted variation of α with K. A proposed mechanism involving successive electron transfer, proton transfer and electron transfer, with metastable intermediates between the steps, is excluded. Such a mechanism would lead to values of k below those predicted by the theory.
ST hydride transfer NAD analog; pyridinium deriv hydride transfer
IT Kinetics of hydride transfer
(between NAD analogs)
IT Redox reaction
(between NAD analogs, equilibrium consts. of)
IT Hydride transfer
(nondegenerate, between NAD analogs, equilibrium consts. of)
IT 53-84-9
RL: PRP (Properties)
(hydride transfer between analogs of)
IT 13367-81-2 16183-83-8 33718-28-4 46176-64-1 85289-84-5
85289-86-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride transfer of, degenerate and nondegenerate, rate and equilibrium consts. of)
IT 85289-80-1 85289-81-2 85289-83-4 87513-45-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride transfer of, degenerate, with undeuterated analog, kinetics of)
IT 87513-46-0 **87513-47-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride transfer of, degenerate, with unfluorinated analog, kinetics of)
IT 38559-35-2 47072-02-6 47136-25-4 84811-85-8 85289-85-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride transfer of, nondegenerate, rate and equilibrium consts. of)
IT **87513-47-1**

RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride transfer of, degenerate, with unfluorinated analog, kinetics of)
RN 87513-47-1 HCAPLUS
CN Pyridinium, 1-[(4-fluorophenyl)methyl]-3-[[(phenylmethyl)amino]carbonyl]-(9CI) (CA INDEX NAME)

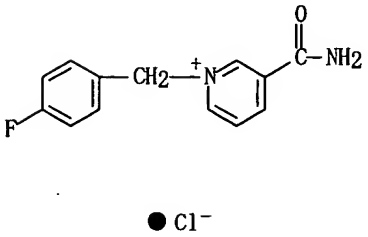


L17 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:504507 HCAPLUS
DN 99:104507
ED Entered STN: 12 May 1984
TI Dihydropyridines. XLVIII. Substituent effect in addition of cyanide ion to p-substituted 1-benzyl-3-carbamoylpyridinium chlorides
AU Pavlikova-Raclova, Frantiska; Kuthan, Josef
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (**1983**), 48(5), 1401-7
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
GI



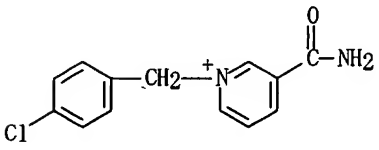
AB Rate consts. for the title reaction were determined in aqueous solns. of 8 quaternary salts of nicotinamide (I; R = p-XC6H4CH2; X = MeO, Me, H, F, Cl, CO2Me, cyano, NO2). Good Hammett correlations were found, along with correlation of E1/2 of polarog. reduction of I with rate and equilibrium consts. In aqueous media, reduction of I (same R; X = Me, H, F, Cl, MeO) with π-donor substituents proceeds via a simple E mechanism I → II, whereas in the case of π-acceptor substituents (I; X = NO2, CN, CO2Me), radicals II are formed via a 3-step CEC mechanism.
ST cyanation benzylcarbamoylpyridinium kinetics mechanism; LFER cyanation benzylcarboamoylpyridinium
IT Linear free energy relationship
(in cyanation of benzylcarbomoylpyridinium chlorides)
IT Cyanation
(of benzylcarbamoylpyridinium chlorides, mechanism of)
IT Kinetics of cyanation
Reduction, electrochemical
(of benzylcarbomoylpyridinium chlorides)
IT **1652-58-0** 5096-13-9 6621-73-4 **6951-52-6** 52354-19-5 63828-55-7 84354-35-8 84389-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)

(cyanation of, kinetics and mechanism of)
IT **1652-58-0 6951-52-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
RN 1652-58-0 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



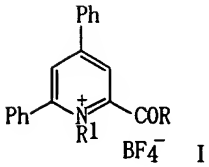
● Cl^-

RN 6951-52-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L17 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:143238 HCAPLUS
DN 98:143238
ED Entered STN: 12 May 1984
TI Intramolecular reactions of pyridinium-2-carbonyl azides: conversion of amines into aldehydes
AU Katritzky, Alan R.; Siddiqui, Tayyaba
CS Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1982**), (12), 2953-6
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 25
OS CASREACT 98:143238
GI



I

AB Pyridinium salts I [R = N3, R1 = CH2C6H4R2-p (R2 = H, Cl, Me)], prepared from I (R = OEt, R1 as before) by sequential treatment with N2H4 and HONO,

on photolysis in CH2Cl2 gave p-R2C6H4CHO in 70-76% yield via γ-lactone intermediates. Similarly, I [R = N3, R1 = (CH2)2Ph] on photolysis gave a 2:1 mixture of PhCHO and PhCH2CHO via the δ- and γ-lactone, resp.

ST benzylazidocarbonylpyridinium photolysis; arylcarboxaldehyde; aldehyde aryl; benzaldehyde; phenylacetaldehyde; pyridinium benzyl azidocarbonyl photolysis

IT Photolysis
(of pyridiniumcarbonyl azides, aldehydes by)

IT Aldehydes, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, through photolysis of pyridiniumcarbonyl azides)

IT Azides
RL: SPN (Synthetic preparation); PREP (Preparation)
(pyridiniumcarbonyl, preparation and photolysis of, aldehyde by)

IT 4224-87-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with Et pyruvate)

IT 617-35-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with methylchalcone)

IT 78904-86-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with amines, pyridinium salts by)

IT 62-53-3, reactions 64-04-0 75-31-0, reactions 100-46-9, reactions 104-84-7 104-86-9 108-91-8, reactions 109-73-9, reactions 156-41-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with pyrylium salt, pyridinium salt by)

IT 85124-78-3P **85124-80-7P** 85124-82-9P 85124-84-1P
85124-86-3P 85124-88-5P 85124-90-9P 85124-92-1P 85124-94-3P
85124-96-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and azidation of)

IT 80560-58-3P 80560-60-7P 80560-64-1P 80560-66-3P 80560-72-1P
80560-74-3P 80572-09-4P 85124-72-7P 85124-74-9P 85124-76-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation reaction of, with hydrazine)

IT 85124-70-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reactions of, with amines, pyridium salts by)

IT 85124-98-7P **85125-00-4P** 85125-02-6P 85125-04-8P
85125-06-0P 85125-08-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photolysis of, aldehyde by)

IT 80575-97-9P 85125-10-6P 85125-12-8P 85125-14-0P 85125-16-2P
85125-17-3P 85125-18-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 100-52-7P, preparation 104-87-0P 104-88-1P, preparation 122-78-1P
123-72-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, through photolysis of pyridiniumcarbonyl azide)

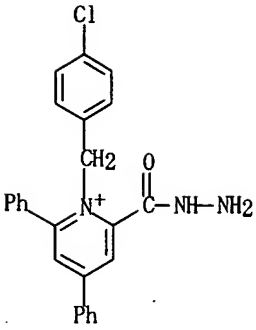
IT **85124-80-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and azidation of)

RN 85124-80-7 HCAPLUS

CN Pyridinium, 1-[(4-chlorophenyl)methyl]-2-(hydrazinocarbonyl)-4,6-diphenyl-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

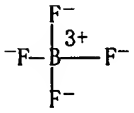
CM 1

CRN 85124-79-4
CMF C25 H21 Cl N3 O



CM 2

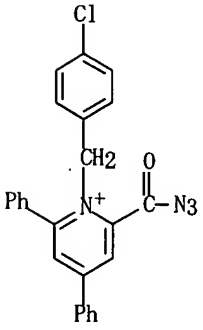
CRN 14874-70-5
CMF B F4
CCI CCS



IT **85125-00-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and photolysis of, aldehyde by)
RN 85125-00-4 HCAPLUS
CN Pyridinium, 2-(azidocarbonyl)-1-[(4-chlorophenyl)methyl]-4,6-diphenyl-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

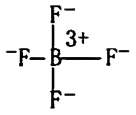
CM 1

CRN 85124-99-8
CMF C25 H18 Cl N4 O

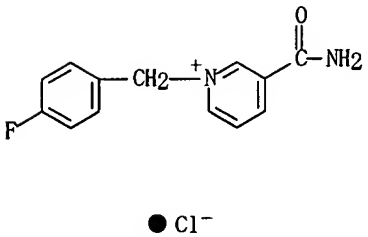


CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

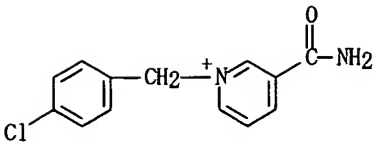


L17 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:61940 HCAPLUS
DN 98:61940
ED Entered STN: 12 May 1984
TI Polarographic reduction of p-substituted 1-benzyl-3-carbamoylpyridinium chlorides
AU Kuthan, Josef; Pavlikova-Raclova, Frantiska
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (**1982**), 47(11), 2890-903
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 72-2 (Electrochemistry)
AB Substituent effects (H, NO2, CN, CO2Me, Me, MeO, Me2N, Cl, F) on polarog. characteristics of the title quaternary salts were studied in H2O, anhydrous MeCN, and aqueous EtOH. In the last solvent, 1 of the polarog. waves gradually disappears. The probable course of the investigated electrode processes and accompanying chemical transformations is discussed.
ST polarog redn benzyl carbamoylpyridinium chloride; quaternary nicotinamide chloride polarog redn
IT Substituent effect
(in polarog. reduction of benzylcarbamoylpyridinium chlorides)
IT Reduction, electrochemical
(of benzylcarbamoylpyridinium chloride p-substituted derivs.)
IT **1652-58-0** 5096-13-9 6621-73-4 **6951-52-6** 52354-19-5 63828-55-7 84354-35-8 84389-20-8 84389-21-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)
IT **1652-58-0 6951-52-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)
RN 1652-58-0 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, chloride (9CI). (CA INDEX NAME)



● Cl⁻

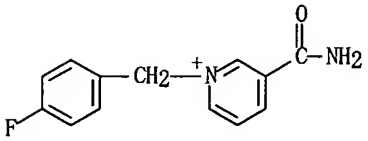
RN 6951-52-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



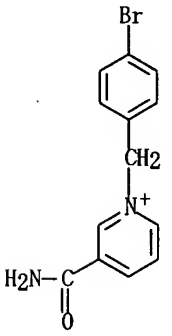
● Cl^-

L17 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1981:549448 HCAPLUS
DN 95:149448
ED Entered STN: 12 May 1984
TI Kinetics and mechanism of the reaction of 5-nitroisoquinolinium cations with 1,4-dihydronicotinamides
AU Bunting, John W.; Sindhuatmadja, Shinta
CS Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.
SO Journal of Organic Chemistry (**1981**), 46(21), 4211-19
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 22-3 (Physical Organic Chemistry)
AB D isotope effects for the title reactions clearly indicate that these are mainly primary kinetic isotope effects and that C-H bond-breaking occurs during the rate-determining transition state for these H transfer reactions. NMR studies show that the H atom is transferred directly to the isoquinolinium cation without exchange with solvent protons. LFER data indicate that the migrating H atom bears -0.44 charge in the transition state and is thus clearly hydridic in character.
ST nitroisoquinolinium dehydronicotinamide reaction mechanism; kinetics reaction nitroisoquinolinium dehydronicotinamide; isotope effect reaction nitroisoquinolinium dehydronicotinamide; LFER reaction nitroisoquinolinium dihydronicotinamide
IT Linear free energy relationship
(in exchange reaction between nitroisoquinolinium ions and dihydronicotinamides)
IT Isotope effect
(in hydrogen exchange between nitroisoquinolinium ions and dihydronicotinamides, by deuterium)
IT Kinetics of exchange reaction
(of hydrogen, between nitroisoquinolinium ion and dihydronicotinamides)
IT Exchange reaction
(of hydrogen, between nitroisoquinolinium ions and dihydronicotinamides, mechanism of)
IT 1333-74-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(exchange reaction of, between nitroisoquinolinium ions and dihydronicotinamides)
IT 7782-39-0, properties
RL: PRP (Properties)
(isotope effect of, in hydrogen exchange between nitroisoquinolinium ions and dihydronicotinamides)
IT 952-92-1 1893-57-8 56133-27-8 56133-29-0 78186-17-1 78186-18-2 78186-19-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitroisoquinolinium cations reduction by)
IT 16183-83-8P 17750-24-2P 60172-94-3P 69337-15-1P 78186-16-0P 78186-22-8P **78186-23-9P 78186-24-0P** 78186-25-1P 78186-26-2P 78186-27-3P 78186-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 52047-79-7
RL: PRP (Properties)
(propyldihydronicotinamide from)
IT 100-39-0 104-81-4 402-49-3 456-41-7 459-46-1 589-15-1

17201-43-3 28188-41-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nicotinamide)
IT 98-92-0
RL: PRP (Properties)
(reaction with benzyl bromide derivative)
IT 52166-52-6 64840-42-2 64840-43-3 64840-44-4 64840-45-5
64840-46-6 78186-20-6 78186-21-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by dehydronicotinamides)
IT 46271-32-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by dihydronicotinamide derivative)
IT **78186-23-9P 78186-24-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78186-23-9 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

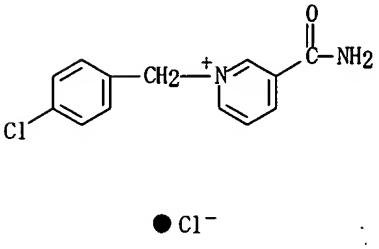


RN 78186-24-0 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-bromophenyl)methyl]- (9CI) (CA INDEX NAME)



L17 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1975:605528 HCAPLUS
DN 83:205528
ED Entered STN: 12 May 1984
TI Function of pyridinium salts on the rate of autoxidation of hydroquinone and its derivatives
AU Shirai, Masamitsu; Koizumi, Taizo; Iguchi, Yoshio; Tanaka, Makoto
CS Fac. Eng., Univ. Osaka Prefect., Sakai, Japan
SO Chemistry Letters (**1975**), (9), 915-18
CODEN: CMLTAG; ISSN: 0366-7022
DT Journal
LA English
CC 22-5 (Physical Organic Chemistry)
AB Autoxidations of hydroquinone and its derivs. are catalyzed by pyridinium salts positively or negatively depending on the properties of the substituents of the pyridinium rings. Formation of charge-transfer complexes between hydroquinones and pyridinium salts plays an important role.
ST hydroquinone autoxidn pyridinium salt; oxidn hydroquinone pyridinium salt

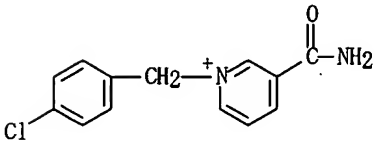
IT Oxidation
(auto-, of hydroquinones, effect of pyridinium salts on)
IT Kinetics of oxidation
(auto-, of hydroquinones, effect pyridinium salts on)
IT Oxidation catalysts
(pyridinium salts, for hydroquinones)
IT 95-71-6 123-31-9, reactions 1948-33-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(autoxidn. of, effect of pyridinium salts on)
IT 2876-13-3 5096-13-9 **6951-52-6** 14535-08-1 16183-82-7
16214-99-6 19432-56-5
RL: PRP (Properties)
(effect of, on autoxidn. of hydroquinone)
IT **6951-52-6**
RL: PRP (Properties)
(effect of, on autoxidn. of hydroquinone)
RN 6951-52-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl^-

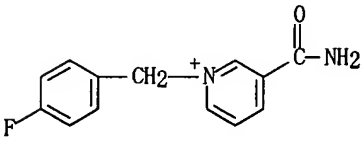
L17 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:552204 HCAPLUS
DN 81:152204
ED Entered STN: 12 May 1984
TI Quaternary pyridinium salts. III. Reactions of quaternary salts of nicotinamide with strong bases
AU Guendel, Wolf H.; Buecher, Bodo; Hagedorn, Ilse
CS Chem. Lab., Univ. Freiburg, Freiburg/Br., Fed. Rep. Ger.
SO Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie, Biochemie, Biophysik, Biologie (**1974**), 29(7/8), 556-60
CODEN: ZENBAX; ISSN: 0044-3174
DT Journal
LA German
CC 28-25 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27
GI For diagram(s), see printed CA Issue.
AB Four mols. of quaternary nicotinamide salts I (R = e.g. Me2CHOCH2, cyclohexyloxymethyl, Et, Me3C, or 4-FC6H4CH2) were condensed reversibly in the presence of stoichiometric amts. of EtONa in EtOH to give the condensates II in varying amts. depending mainly on the electron-donating effects of R. Electron-attracting R (e.g. 4-O2NC6H4) inhibited II formation, favoring the known deprotonation of the methylene group.
ST quaternary nicotinamide salt condensation
IT 2254-97-9P 5096-13-9P 6621-73-4P **6951-52-6P** 14596-52-2P
20764-51-6P 53406-00-1P 54027-55-3P 54027-56-4P 54027-57-5P
54027-58-6P 54027-59-7P 54027-60-0P 54071-90-8P
54071-91-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, cyclic tetramer from)
IT 53164-19-5P 54027-61-1P 54027-62-2P 54027-63-3P 54027-64-4P
54027-65-5P 54027-66-6P 54027-67-7P 54027-68-8P 54027-69-9P
54027-70-2P 54071-92-0P 54071-93-1P 54144-68-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 98-92-0
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, salts from)
IT **6951-52-6P 54027-58-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and condensation of, cyclic tetramer from)
RN 6951-52-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

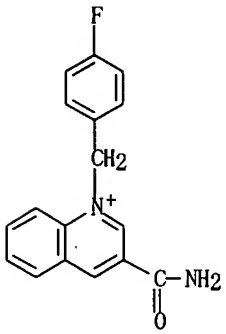
RN 54027-58-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, bromide (9CI) (CA INDEX NAME)



● Br^-

L17 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1969:512781 HCAPLUS
DN 71:112781
ED Entered STN: 12 May 1984
TI Mechanism of reduction of 3-carboxamidoquinolinium salts with formic acid and triethylamine
AU Gizzi, Leo R.; Joullie, Madeleine M.
CS Univ. of Pennsylvania, Philadelphia, PA, USA
SO Tetrahedron Letters (**1969**), (36), 3117-20
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
CC 27 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 71:112781
GI For diagram(s), see printed CA Issue.
AB N-(p-Fluorobenzyl)-3-carboxamidoquinolinium chloride (I), HCO2H, and NEt3 in 1:2:2.5 molar ratio heated 5 hrs. and worked up yielded 80% II, m. 187-9° . Treatment of II with addnl. HCO2H and NEt3 gave N-(p-fluorobenzyl)-1,2,3,4-tetrahydroquinoline (III), Deuteration expts. showed that the reaction involved hydride shifts. N.M.R. data were given and discussed.
ST quinolines salts redn mechanism; salts quinolines redn mechanism; redn mechanism quinolines salts; mechanism redn quinolines salts; deuteration quinolines
IT Reduction
(of carbamoylquinolinium salts, mechanism of)
IT 64-18-6, reactions 121-44-8, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(in reduction of carbamoylquinolinium salts, mechanism of)
IT 23969-92-8P 23969-93-9P 23969-94-0P 23969-95-1P 23969-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
IT **25683-53-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, mechanism of)
IT **25683-53-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, mechanism of)
RN 25683-53-8 HCAPLUS
CN Quinolinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, chloride (9CI)
(CA INDEX NAME)



● Cl⁻

L17 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1968:459060 HCAPLUS
DN 69:59060
ED Entered STN: 12 May 1984
TI Structure and reactivity of the intermediate formed in the sodium dithionite reduction of pyridinium salts
AU Biellmann, Jean-Francois; Callot, Henry Jacques
CS Inst. Chim., Strasbourg, Fr.
SO Bulletin de la Societe Chimique de France (**1968**), (3), 1154-9
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
CC 27 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 69:59060
GI For diagram(s), see printed CA Issue.
AB Salts of the general formula I are treated with Na2S2O4 in the presence of NaOH to give compds. of the general formula II; compds. of the general formula III are prepared from the I in the presence of NaHCO3. Thus, a mixture of nicotinamide, p-ClC6H4CH2Cl, and MeOH is heated to give 1-(p-chlorobenzyl)nicotinamide chloride (IV), m. above >260°. Similarly prepared is I (R = o-ClC6H4CH2), m. 260° (decomposition). A solution of 2 g. I (R = PhCH2) and 10 ml. water is treated with a solution of 2.5 g. Na2S2O4 and 1 g. NaOH in 15 ml. water and the mixture kept 5-10 min. at 10° to give 2.27 g. sodium 1-benzyl-1,4-dihydronicotinamide-4-sulfinate (V), decomposed 140°. Similarly prepared are (decomposition temperature given): II (R = p-ClC6H4CH2) (VI), .apprx.140°; II (R = o-ClC6H4CH2), .apprx.140°. A solution of 500 mg. IV in 35 ml. water is treated with a solution of 500 mg. Na2S2O4 and 1 g. NaHCO3 in 15 ml. water and the mixture kept 2 hrs. at 0° to give 280 mg. 1-(p-chlorobenzyl)-1,4-dihydronicotinamide (VII), m. 130-1°. Similarly prepared is III (R = o-ClC6H4CH2), m. 139-41°. III (R = PhCH2) (VIII), m. 122-4°, is prepared according to D. Mauzerall and F. H. Westheimer (1955). IV is reduced in D2O to give VII-4-d which is treated with Ag2O to give IV-4-d0.5; IV-4-d0.5 is treated with Na2S2O4 to give VI-4-d0.5. The aqueous hydrolysis of 100 mg. V under N gives 52% VIII, m. 122-3°. The II are hydrolyzed with pyridinium salts to give the corresponding III. N.M.R. data for the II and III and ir data for the II are given. IX (Ar = 2,6-Cl2C6H3, R = CN, X = Br), IX (Ar = PhCH2, R = Ac,

X = Cl), X (Ar = 2,6-Cl2C6H3, R = CN), and X (Ar = PhCH2, R = Ac) are prepared according to known methods.

ST dithionites redn pyridinium salts; pyridinium salts dithionites redn; redn pyridinium salts dithionites

IT Reduction
(of pyridinium compds., by sodium dithionite, reactivity of intermediate in)

IT Pyridinium compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by sodium dithionite, reactivity of intermediate in)

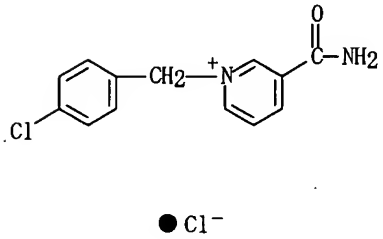
IT 632-93-9P 952-92-1P 1149-23-1P 5096-12-8P 5096-13-9P
6951-52-6P 10538-16-6P 13014-55-6P 13014-56-7P 19350-51-7P
19350-55-1P 19350-56-2P 19350-59-5P 19350-64-2P 19350-66-4P
19350-67-5P 19355-20-5P 19650-91-0P 20991-42-8P 21641-56-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 7775-14-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyridinium compds. reduction by, reactivity of intermediate and)

IT **6951-52-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 6951-52-6 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L17 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1963:454780 HCAPLUS

DN 59:54780

OREF 59:**9970a-c**

ED Entered STN: 22 Apr 2001

TI Action of base on quaternary salts of nicotinamide

AU Dittmer, Donald C.; Kolyer, J. M.

CS Univ. of Pennsylvania, Philadelphia

SO Journal of Organic Chemistry (**1963**), 28(9), 2288-94
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA Unavailable

CC 37 (Heterocyclic Compounds (One Hetero Atom))

GI For diagram(s), see printed CA Issue.

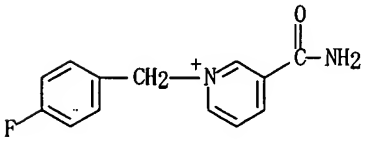
AB Treatment of 1benzyl-3-carbamoylpyridinium chloride with NaOH in dilute EtOH yielded a new substance (I), believed to be a cyclic trimer. The structure of I was based on its analysis, infrared spectrum, ultraviolet spectrum, fluorescence spectrum, proton magnetic resonance spectrum, mol. weight, and its chemical reactions. I is believed to have been formed by way of a pyridinium ylide. Several new pseudo base ethers of 1-substituted nicotinamide salts have been prepared

IT Spectra, visible and ultraviolet
(of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]-heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)

IT Spectra, infrared
(of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)

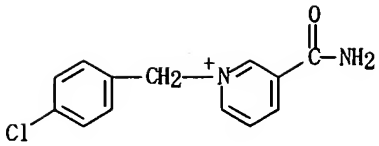
IT Nuclear magnetic resonance
(of 1,6,11-triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)

IT Bases
(reactions of, with 3-carbamoylpyridinium derivs.)
IT Nitrone, α-benzyl-N-[p-(dimethylamino)phenyl]-α-phenyl-
IT Pyridinium, 3-carbamoyl-
(derivs., reaction with bases)
IT 952-92-1, Nicotinamide, 1-benzyl-1,4-dihydro- **1652-58-0**, Pyridinium, 3-carbamoyl-1-(p-fluorobenzyl)-, chloride 1893-57-8, Nicotinamide, 1-(p-fluorobenzyl)-1,4-dihydro- 2996-08-9, Nicotinamide, 4,4'-oxybis[1-(p-fluorobenzyl)-1,4-dihydro- 4533-64-6, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-fluorophenyl)- 5096-13-9, Pyridinium, 1-benzyl-3-carbamoyl-, chloride 6621-73-4, Pyridinium, 3-carbamoyl-1-(p-nitrobenzyl)-, chloride **6951-52-6**, Pyridinium, 3-carbamoyl-1-(p-chlorobenzyl)-, chloride 13502-54-0, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,4-dihydro- 19355-18-1, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,6-dihydro- 63828-55-7, Pyridinium, 3-carbamoyl-1-(p-methoxybenzyl)-, chloride 75340-29-3, Nicotinamide, 4,4'-oxybis[1-benzyl-1,4-dihydro- 92578-90-0, Glycine, N-(p-tolylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93807-08-0, Glycine, N-(phenylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93946-35-1, Glycine, N-(p-tolylsulfonyl)-, 2-(m-bromophenyl)hydrazide 94379-06-3, Nipecotamide, 1-benzyl-, picrate 95945-13-4, Nicotinamide, 4,4'-oxybis[1,4-dihydro-1-(p-nitrobenzyl)- 96003-72-4, Nicotinamide, 4,4'-oxybis[1-(2,6-dichlorobenzyl)-1,4-dihydro- 96635-71-1, Nipecotamide, 1-benzyl-, hydrochloride 96650-48-5, Pyridinium, 3-carbamoyl-1-(2,4-dinitrobenzyl)-, chloride 98310-77-1, Pyridinium, 1-benzyl-3-carbamoyl-, oxalate 100210-41-1, Pyridinium, 1-benzyl-3-carbamoyl-, picrate 106141-61-1, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-bromophenyl)- 106141-62-2, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-chlorophenyl)- 106141-68-8, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-triphenyl- **106384-38-7**, Pyridinium, 1-(p-bromobenzyl)-3-carbamoyl-, chloride
(preparation of)
IT **1652-58-0**, Pyridinium, 3-carbamoyl-1-(p-fluorobenzyl)-, chloride
6951-52-6, Pyridinium, 3-carbamoyl-1-(p-chlorobenzyl)-, chloride
106384-38-7, Pyridinium, 1-(p-bromobenzyl)-3-carbamoyl-, chloride
(preparation of)
RN 1652-58-0 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-fluorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



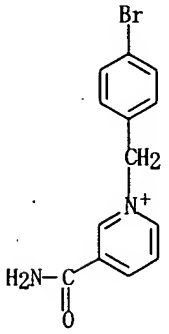
● Cl^-

RN 6951-52-6 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-chlorophenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

RN 106384-38-7 HCAPLUS
CN 1-(p-Bromobenzyl)-3-carbamoylpyridinium chloride (7CI) (CA INDEX NAME)



● Cl⁻

L17 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1963:454779 HCAPLUS
DN 59:54779
OREF 59:**9969g-h, 9970a-c**
ED Entered STN: 22 Apr 2001
TI The reaction of cyanomethyl esters of carboxylic acids with arylhydrazines. III. Investigation of the influence of bromine substituents in the benzene ring of phenylhydrazine on the acylation reaction by cyanomethyl carboxylates
AU Grudzinska, P.
CS Univ. Lodz, Pol.
SO Lodz. Towarz. Nauk, Wydzial III, Acta Chim. (**1962**), 8, 131-40
DT Journal
LA English
CC 37 (Heterocyclic Compounds (One Hetero Atom))
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 16478i. oBrC6H4NHNH2.HCl, m. 184-5° (decomposition) (1:4 HCl-H2O), dissolved in hot H2O, basified with 3N KOH, and cooled yielded. o-BrC6H4NHNH2 (I), needles, m. 46-8° . Similarly were prepared the m-isomer of I, straw-colored oil, b.-, 132-5D b20 174-6° , 53%, and the light yellow p-isomer of I, m. 105-77, 50% [HCl salt m. 201 3° (decomposition)]. The appropriate cyanomethyl ester (0.005 mole)4 and 0.006 mole of a suitable bromophenylhydrazine in 10 cc. EtOAc refluxed 9 (or 20 hrs.) yielded the corresponding RCONHNHC6H4Br (II); in this manner were prepared the following II (with o-Br)(R, % crude yield, and m.p. given): BzNHCH2, 61, 184-5° (absolute EtOH) (71% during 20 hrs.); Ph-SO2NHCH2, 50, 130-1° (98% EtOH) (73% during 20 hrs.); pMeC6H4SO2NHCH2, 64.3, 121-3° (96% EtOH) (73.5% during 20 hrs.); 4-pyridyl, 27.4 (during 20 hrs.), 169-70° (EtOH). In the same manner were prepared the following II (with m-Br) (same data given): BzNHCH2, 88, 197 8° (EtOH); PhSO2-NHCH2, 84, 159 60° (EtOH); p-MeC6H4SO2NHCH2, 69.4, 154-5° (EtOH); 4-pyridyl, 48.5 (during 20 hrs.), - [HCl salt m. 261-3° (decomposition) (50% AcOH)]; and the following II (with p-Br)

(same data given): BzNHCH2, 93, 213-15° (decomposition) (50% AcOH); PhSO2NHCH2, 100, 186-7° (decomposition) (96% EtOH); p-MeC6H4SO2NHCH2, 91, 195 6° (decomposition) (EtOH); 4-pyridyl, 42.5 (during 20 hrs.), - [HCl salt, yellow needles, m. 215° (decomposition) (aqueous HCl)].

IT Acylation
(by glycolonitrile esters)

IT Hydrazine, (m-bromophenyl)-
Nitrone, α-benzyl-N-[p-(dimethylamino)phenyl]-α-phenyl-

IT 302-01-2, Hydrazine
(aryl derivs., reaction with glycolonitrile esters)

IT 100-63-0, Hydrazine, phenyl-
(derivs., in acylation by glycolonitrile esters)

IT 110-94-1, Glutaric acid
(derivs., reaction with 3-(2-aminoethyl)indole)

IT 75-05-8, Acetonitrile
(esters)

IT 107-16-4, Glycolonitrile
(esters, reaction with arylhydrazines)

IT 7726-95-6, Bromine
(in acylation by glycolonitrile esters)

IT 589-21-9, Hydrazine, (p-bromophenyl)- 4533-64-6, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-fluorophenyl)- 16732-66-4, Hydrazine, (o-bromophenyl)- 50709-33-6, Hydrazine, (o-bromophenyl)-, hydrochloride 91912-33-3, Succinimide, N-[(dimethylamino)methyl]-, hydrochloride 92425-57-5, Hippuric acid, 2-(o-bromophenyl)hydrazide 92576-81-3, Isonicotinic acid, 2-(o-bromophenyl)hydrazide 92578-89-7, Glycine, N-(p-tolylsulfonyl)-, 2-(o-bromophenyl)hydrazide 92578-90-0, Glycine, N-(p-tolylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93807-06-8, Glycine, N-(phenylsulfonyl)-, 2-(m-bromophenyl)hydrazide 93807-07-9, Glycine, N-(phenylsulfonyl)-, 2-(o-bromophenyl)hydrazide 93807-08-0, Glycine, N-(phenylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93897-68-8, Hippuric acid, 2-(m-bromophenyl)hydrazide 93897-69-9, Hippuric acid, 2-(p-bromophenyl)hydrazide 93946-35-1, Glycine, N-(p-tolylsulfonyl)-, 2-(m-bromophenyl)hydrazide 94379-06-3, Nipecotamide, 1-benzyl-, picrate 95592-93-1, Isonicotinic acid, 2-(m-bromophenyl)hydrazide, hydrochloride 95592-94-2, Isonicotinic acid, 2-(p-bromophenyl)hydrazide, hydrochloride 96635-71-1, Nipecotamide, 1-benzyl-, hydrochloride 106141-61-1, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-bromophenyl)- 106141-62-2, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-chlorophenyl)- 106141-68-8, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-triphenyl-
(preparation of)

IT 61-54-1, Indole, 3-(2-aminoethyl)-
(reaction with glutaric acid derivs.)

L17 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1960:23099 HCAPLUS
DN 54:23099
OREF 54:**4573f-i**
ED Entered STN: 22 Apr 2001
TI The mechanism of hydrogen transfer with pyridine nucleotides. XVI. A third type of dihydropyridine isomer of nicotinamide
AU Wallenfels, Kurt; Schuly, Hans
CS Univ. Freiburg, Germany
SO Ann. (**1959**), 621, 215-21
DT Journal
LA Unavailable
CC 10G (Organic Chemistry: Heterocyclic Compounds)
AB With H2S, malonic acid dinitrile was converted to cyanothioacetamide which was condensed with acetylacetone to 2,4-dimethyl-5-cyano-6-mercaptopyridine. Methylation with Me2SO4 and treatment with Zn gave 2,4-dimethyl-5-cyanopyridine which on treatment with NH3 and H2O2 in acetone gave 90% 4,6-dimethylnicotinamide (I), m. 164-5° . After refluxing 7.5 g. I with 12 g. 2,6-dichlorobenzyl bromide in 50 ml. MeOH 2 hrs. and cooling, 200 ml. Et2O was added in small portions. After 6 hrs. the mixture was filtered to give 18 g. N1-(2,6-dichlorobenzyl)-4,6-dimethylnicotinamide bromide (II), m. 236-8° (decomposition) (H2O).

This hygroscopic material crystallized with 2 moles H2O. After 14 hrs. drying in vacuo at 65° over P2O5, only 1 mole H2O was present. Reduction of II with Na2S2O4 in Na2CO3 gave 50-60% crystalline product, m. above 150° (MeOH), λ (ε in cc./mmole) 392 mμ (4690). In neutral solution AgNO3 was reduced instantly. Reduction with NaBH4 and Na2CO3 gave 96% crystalline product with properties identical to those of the Na2S2O4 reduction product. Comparison of the absorption spectra of this compound with previously prepared reduction products (cf. part XI) indicated that this compound was a 1,2-dihydropyridine.

IT Ultraviolet and visible, spectra
(of 1-(2,6-dichlorobenzyl)-1,2-dihydro-4,6-dimethylnicotinamide)

IT 6623-21-8, Nicotinonitrile, 4,6-dimethyl- 7357-70-2, Acetamide, 2-cyanothio- 13061-58-0, Nicotinamide, 4,6-dimethyl- 19340-27-3, Pyridinium, 5-carbamoyl-1-(2,6-dichlorobenzyl)-2,4-dimethyl-, bromide 19355-15-8, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,2-dihydro-4,6-dimethyl- 54585-47-6, Nicotinonitrile, 2-mercapto-4,6-dimethyl- 106472-13-3, Isonicotinamide, 1-(2,6-dichlorobenzyl)-1,6-dihydro- 106472-33-7, Isonicotinamide, 1-(2,6-dichlorobenzyl)-1,4-dihydro-
(preparation of)

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L12 ANSWER 1 OF 2 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA59:9970a CAOLD
TI action of base on quaternary salts of nicotinamide
AU Dittmer, Donald C.; Kolyer, J. M.
IT 952-92-1 **1652-58-0** 1893-57-8 2996-08-9 4533-64-6
5096-13-9 6621-73-4 **6951-52-6** 13502-54-0 19355-18-1
63828-55-7 75340-29-3 92578-90-0 93807-08-0 93897-69-9 93946-35-1
94379-06-3 95592-93-1 95592-94-2 95945-13-4 96003-72-4 96635-71-1
96650-48-5 98310-77-1 100210-41-1 106141-61-1 106141-62-2 106141-68-8
106384-38-7

L12 ANSWER 2 OF 2 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA54:4573g CAOLD
TI mechanism of H transfer with pyridine nucleotides - (IX) pyridinium salts and dihydropyridine as model substances of dephosphopyridine nucleotide and reduced diphosphopyridine nucleotide
AU Wallenfels, Kurt; Schuely, H.; Hofmann, D.
IT 6623-21-8 7357-70-2 13061-58-0 54585-47-6 **132778-91-7**

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L12 ANSWER 1 OF 2 HCAOLD COPYRIGHT 2005 ACS on STN
CA59:9970a

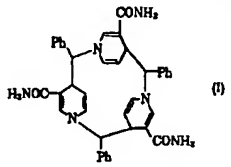
<CAOld PAGE IMAGE BYTES 153010>

p-MeC_6H_4, 96, 183–6°/0.15, 1.6089; Bu, $PhCH_2$, 83, 183–5°/0.20, 1.6051; Pr, $PhCH_2$, 87, 183–4°/0.1, 1.6117; Pr, *p*-$PrOC_6H_4CH_2$, —, 204–10°/0.02, —; Pr, 2-(2-pyridylethyl), —, 206–7°/0.15, 1.6029. C_6Cl_5OH (5.32 g.) in 50 cc. EtOH treated with 0.8 g. NaOH and then slowly with stirring dropwise with 3.73 g. III, stirred 5 hrs. at 60–70°, and cooled yielded 6.3 g. 3,4-Me(MeS)$C_6H_3CH_2OC_6Cl_5$, needles, m. 142° (EtOH). Similarly were prepd. the following 3,4-Me(RS)$C_6H_3CH_2OC_6Cl_5$ (R, % yield, and m.p. given): Et, 63, 91°; Pr, 75, 94°; Bu, 73, 96°. In the same manner were prepd. the following 3,4-Me(RS)$C_6H_3CH_2SC_6Cl_5$ (same data given): Et, 57, 111°; Pr, 65, 96°; Bu, 61, 80°. VI (21.5 g.) added slowly to 9.8 g. KSCN, refluxed 3 hrs., dild. with H_2O, and extd. with Et_2O yielded 21.7 g. 3,4-Me(PrS)$C_6H_3CH_2SCN$, $b_{0.5}$ 147.5–51°, n_D^{25} 1.6063. VI (53.8 g.) in 200 cc. Me_2CO added dropwise slowly with stirring to 44 g. KCN in 100 cc. H_2O and 6.2 g. NaI in 10 cc. H_2O, refluxed about 15 hrs., filtered, and evapd., and the residue dissolved in Et_2O and worked up gave 37.2 g. II, $b_{0.04}$ 137–9°, n_D^{25} 1.5620. II (20.5 g.) in 100 cc. Et_2O added dropwise to 3.8 g. $LiAlH_4$ in 150 cc. dry Et_2O at such a rate as to maintain reflux yielded 21 g. I, $b_{0.01}$ 113–15°, n_D^{25} 1.5659; I.HCl, needles, m. 74°. F. W. Hoffmann

Carboxylic acid esters of α-dialkylaminoalkanols. Horst Boehme, Hans Joachim Bohn, Ernst Koehler, and Juergen Roehr (Univ. Marburg, Ger.). *Ann. Chem.* 664, 130–40(1963). Acid anhydrides and aminals, $RCH(NR_2)_2$, or α-dialkylamino ethers yielded the title compds. (I), which with acid chlorides or HCl gave α-chloroamines. I with some strong acids gave methylenimmonium salts, $[R_2N^+{:}CH_2 \leftrightarrow R_2NC^+H_2]Y^-$. Several condensation products were prepd. from I and active H compds. The product obtained from $Et_2NCH_2SO_3Na$ and Ac_2O and reported to be Et_2NCH_2OAc [Knoevenagel and Mercklin, *Ber.* 37, 4087–94(1904)] was shown to be a mixt. of $AcNEt_2$ ($HAuCl_4$ adduct m. 56°) and $CH_2(OAc)_2$. $CH_2(NMe_2)_2$ (20.4 g.) with 20.4 g. Ac_2O (below 60°) gave 92% Me_2NCH_2OAc (II), b_{44} 48–50°, n_D^{25} 1.4120, and Me_2NAc. Similarly prepd. were [compd., b.p. (mm.), n_D^{25}, and % yield listed]: Et_2NCH_2OAc (III), 63–4° (20), 1.4226 (21°), 85; pyrrolidinomethyl acetate, 40–1° (1), 1.4450 (21°), 73; morpholinomethyl acetate, 88–9° (3), 1.4527, 82; piperidinomethyl acetate (IV), 55–7° (1), 1.4506, 67; Bu_2NCH_2OAc, 76° (0.2), —, 82; $PhCH_2NMeCH_2OAc$, 71–3° (0.04), —, 75; α-piperidinobenzyl acetate (V), 76–80° (0.01) (bath temp.), 1.5099, 54; Me_2NCH_2OBz, 108° (2), 1.5400, 89. Piperidinomethyl butyl ether (VI) and Ac_2O gave 88% IV. Heating III at 80° yielded $AcNEt_2$ and CH_2O. $AcNMeCH_2Ph$ $b_{0.1}$ 88–90°, m. 43°. By the method of Mannich and Davidsen (*CA* 30, 8217²), VI and Ac_2O yielded 62% 1-piperidino-1-isobutene, b_{17} 65°, which in ether with HCl gave *N*-(α-chloroisobutyl)piperidine. II and CCl_3CO_2H or CCl_3COF in ether gave 89% *N*,*N*-dimethyl-*N*-methylenimmonium trichloroacetate. *N*-Methylenepiperidinoimmonium trichloroacetate (85%) was prepd. similarly. V and AcCl in ether gave 95% *N*-(α-chlorobenzyl)piperidine. Et_2NCH_2Cl and *N*-(chloromethyl)-pyrrolidine were also prepd. I in CCl_4 were condensed with $MeCH(CO_2Et)_2$, PhAc, PhC:CH, $PhNMe_2$, or succinimide, usually by refluxing 2–3 hrs. Compds. obtained were [product, b.p. (mm.), n_D^{25}, and % yield listed]: Et (piperidinomethyl)-methylmalonate, 150–1° (10), 1.4551 (21°), 49; $Me_2NCH_2C(CO_2Et)_2Me$, 118–19° (10), 1.4330, 55; β-piperidinopropiophenone, 70–3° (0.01) (bath temp.), 1.5341 (21°), 38; $Me_2N(CH_2)_2Bz$, — (hydrochloride m. 156°), —, 62; $Et_2NCH_2C{:}CPh$, 137° (hydrochloride m. 136°), —, 50; $Me_2NCH_2C{:}CPh$, 124° (20) (hydrochloride m. 156°), 1.5430 (21°), 78; 4-$Me_2NC_6H_4CH_2NMe_2$, 134° (12), 1.5419, 31; *N*-(morpholinomethyl)succinimide, — (m. 111–12°), —, 60; *N*-(dimethylaminomethyl)-succinimide (VII), 112–14° (2) (m. 45°), —, 75. Heating 10.0 g. succinimide, 3.0 g. paraformaldehyde, and 15.0 g. 33% Me_2NH gave 68% VII; hydrochloride m. 139°. C. M. Buess

The reaction of cyanomethyl esters of carboxylic acids with arylhydrazines. III. Investigation of the influence of bromine substituents in the benzene ring of phenylhydrazine on the acylation reaction by cyanomethyl carboxylates. P. Grudzinska (Univ. Lodz, Poland). *Lodz. Towarz. Nauk, Wydział III, Acta Chim.* 8, 131–40(1962)(in English); cf. *CA* 57, 16478*i*. *o*-$BrC_6H_4NHNH_2.HCl$, m. 184–5° (decompn.) (1:4 HCl–H_2O), dissolved in hot H_2O, basified with 3*N* KOH, and cooled yielded *o*-$BrC_6H_4NHNH_2$ (I), needles, m. 46–8°. Similarly were prepd. the *m*-isomer of I, straw-colored oil, b_3 132–5°, b_{20} 174–6°, 53%, and the light yellow *p*-isomer of I, m. 105–7°, 50% [HCl salt m. 201–3° (decompn.)]. The appropriate cyanomethyl ester (0.005 mole) and 0.006 mole of a suitable bromophenylhydrazine in 10 cc. EtOAc refluxed 9 (or 20 hrs.) yielded the corresponding $RCONHNHC_6H_4Br$ (II); in this manner were prepd. the following II (with *o*-Br)(R, % crude yield, and m.p. given): $BzNHCH_2$, 61, 184–5° (abs. EtOH) (71% during 20 hrs.); $PhSO_2NHCH_2$, 50, 130–1° (98% EtOH) (73% during 20 hrs.); *p*-$MeC_6H_4SO_2NHCH_2$, 64.3, 121–3° (96% EtOH) (73.5% during 20 hrs.); 4-pyridyl, 27.4 (during 20 hrs.), 169–70° (EtOH). In the same manner were prepd. the following II (with *m*-Br) (same data given): $BzNHCH_2$, 83, 197–8° (EtOH); $PhSO_2NHCH_2$, 84, 159–60° (EtOH); *p*-$MeC_6H_4SO_2NHCH_2$, 69.4, 154–5° (EtOH); 4-pyridyl, 48.5 (during 20 hrs.), — [HCl salt m. 261–3° (decompn.) (50% AcOH)]; and the following II (with *p*-Br) (same data given): $BzNHCH_2$, 93, 213–15° (decompn.) (50% AcOH); $PhSO_2NHCH_2$, 100, 186–7° (decompn.) (96% EtOH); *p*-$MeC_6H_4SO_2NHCH_2$, 91, 195–6° (decompn.) (EtOH); 4-pyridyl, 42.5 (during 20 hrs.), — [HCl salt, yellow needles, m. 215° (decompn.) (aq. HCl)]. F. W. Hoffmann

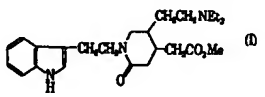
Action of base on quaternary salts of nicotinamide. Donald C. Dittmer and J. M. Kolyer (Univ. of Pennsylvania, Philadelphia). *J. Org. Chem.* 28(9), 2288–94(1963). Treatment of 1-benzyl-3-carbamoylpyridinium chloride with NaOH in dil. EtOH yielded a new substance (I), believed to be a cyclic trimer.



(I)

The structure of I was based on its analysis, infrared spectrum, ultraviolet spectrum, fluorescence spectrum, proton magnetic resonance spectrum, mol. wt., and its chem. reactions. I is believed to have been formed by way of a pyridinium ylide. Several new pseudo base ethers of 1-substituted nicotinamide salts have been prepd. RCKF

Condensation of β-substituted glutaric acids with tryptamine. E. A. Markaryan, R. P. Evstigneeva, and N. A. Preobrazhenskii (M. V. Lomonosov Inst. Fine Chem. Technol., Moscow). *Zh. Obshch. Khim.* 33(4), 1123–7(1963); cf. *CA* 56, 2422*h*. $MeO_2CCH_2CH(CH_2CO_2Me)CH(CN)CH_2CH_2NEt_2$ and tryptamine hydrogenated in MeOH over Raney Ni at 114–16° and 100 atm. 1.5–2 hrs. gave 24.2% Me *N*-(β-3-indolylethyl)-5-*N*′-diethylaminoethylpiperid-2-on-4-ylacetate (I), $b_{0.05}$ 143–7°, which after



(I)

purification on Al_2O_3 in C_6H_6 m. 170–1.5°, λ 280 mμ. Also isolated was 13.5% bis(*N*-3-indolylethyl)amine, $b_{0.05}$ 129–32°, m. 98.5–100° (after chromatography on Al_2O_3); λ 280 mμ. I dipicrate m. 224–6°. Similar hydrogenation of tryptamine with $MeO_2CCH_2CH(CH_2CO_2Me)C(CN)(CO_2Me)CH_2CH_2NEt_2$ (II) gave, after treatment of the crude product in C_6H_6 with aq. K_2CO_3 2 hrs. at 80°, sepn. of unreacted tryptamine, neutralization with HCl, and extn. with BuOH, then heating the product with MeOH in the presence of H_2SO_4 1 hr., 26.4% Me *N*-(β-3-indolylethyl)-5-carbomethoxy-5-*N*′-diethylaminoethylpiperid-2-on-4-ylacetate, $b_{0.05}$ 147–51°, isolated as the dipicrate m. 234–5°, λ 355 mμ; and 2.98% Me 5-carbomethoxy-5-*N*′-diethylaminoethylpiperid-2-on-4-ylacetate (III), $b_{0.15}$ 133–4°, m. 97–8.5°. Hydrogenation of II over Raney Ni as above gave 88.5% III. Hydrogenation of tryptamine with $MeO_2CCH_2CH(CH_2CO_2Me)CH(CN)CH_2CH_2CO_2Bu$ gave 58.5% Me 5-β-carbobutoxyethylpiperid-2-on-4-ylacetate, an oil, λ 280 mμ. G. M. Kosolapoff

Activation of methyl groups on heterocycles. A. N. Kost and A. K. Sheinkman (M. V. Lomonosov State Univ., Moscow). *Zh. Obshch. Khim.* 33(6), 2077–8(1963). The standard method of activating Me groups adjacent to heterocycles with the use of quaternary ammonium iodides (Horwitz, *CA* 50, 2595*h*) is often not suitable as it tends to form *N*-alkylated styryl derivs. The *N*-oxide method (Parker and Furst, *CA* 52, 12866*e*) gives low yields of condensation products. Me groups adjacent to the heterocycle are activated by converting the heterocycle to an *N*-acyl salt by means of a suitable acid chloride. Thus, 4-picoline, treated in the cold with acid chlorides, is easily converted to the corresponding acylpyridinium salts, which react in the cold with aromatic aldehydes (in $HCONMe_2$ soln.). In many cases the acyl group splits off spontaneously as an aldehyde and forms a styryl deriv.; e.g. the salt obtained by treating 4-picoline with BzCl reacts exothermically with *p*-dimethylaminobenzaldehyde and, after brief heating at 150° to complete the reaction, yields up to 70% 4-(*p*-dimethylaminostyryl)pyridine, m. 239–40° (P., *loc. cit.*). Analogous results were obtained with chlorides of acetic, propionic, butyric, hexanoic, isovaleric, *p*-nitrobenzoic, and other acids. The *N*-acyl group activates predominantly the γ-methyl group; expts. carried out under similar conditions with 2-picoline gave only 10–15% yields of 2-(*p*-dimethylaminostyryl)-pyridine. Successful Me group activations were obtained in 2,4-lutidine and in 4-methylquinoline. Andrew L. Grochowski

Synthesis of 2-hydrazinoisonicotinoylhydrazine and its *N*-oxide. A. Martin Municio and A. Ribera (Inst. Quim. Alonso Barba, Madrid). *Anales Real Soc. Espan. Fis. Quim.* (Madrid)

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pyridinium salts. Kurt Wallenfels and Manfred Gellrich (Univ. Freiburg, Ger.). *Ibid.* 198-214.—By titration with Cr(II)Ac the oxidn.-redn. potentials of *N*¹-(2,6-dichlorobenzyl) derivs. of isonicotinic acid bromide (I) and 2,6-dichlorobenzyl(4-substituted)pyridinium bromides were detd. At pH 13, the E_0 values were: I, <1.02; 4-carbomethoxy, <1.02; 4-carbamoyl, −0.849; 4-(4-methyl-2-thiazolyl), −0.864; 4-(4-phenyl-2-thiazolyl), −0.865; 4-(4,5-diphenyl-2-thiazolyl), −0.835; 4-(2-benzothiazolyl), −0.747. *N*¹-(2,6-Dichlorobenzyl)-4-(4-methyl-2-thiazolyl)pyridinium bromide (II) was prepd. by refluxing 10 g. isonicotinic acid thioamide (III) in 50 ml. abs. EtOH with 16 g. bromoacetone. On cooling, the HBr salt of the base, m. 218–20° (EtOH–EtOAc), pptd. After distg. the EtOH from the mother liquor, the resinous residue was taken up in H_2O, filtered, and made alk. with $NaHCO_3$. The isolated base was taken up in Et_2O, dried over NaOH, freed from Et_2O, and the residue sublimed at 140–50°/10 mm. Together with that isolated from the HBr salt, 60% yield of 4-(4-methyl-2-thiazolyl)pyridine, m. 72–3° (m. 69–71°, cf. Bartz, *et al.*, *C.A.* 49, 6952*b*), λ (log ε) 304 mμ (4.06), 225 mμ (3.80) (0.01*M* glycine buffer, pH 9.0), was obtained. This product (1.8 g.) and 2.4 g. 2,6-dichlorobenzyl bromide in Me_2CO gave 72% II, m. 248–50° (MeOH), λ (log ε) 354 mμ (4.28), 293 (3.43), 283 (3.52), 245 (3.83) (H_2O). Similarly 6.5 g. III with 10 g. phenacyl bromide in 100 ml. EtOH gave 43% 4-(4-phenyl-2-thiazolyl)pyridine, m. 113.5–14.5° (dil. EtOH), λ (log ε) 323 mμ (3.95), 245 mμ (4.35) (0.01*M* glycine buffer, pH 9.0, with 50% MeOH). Heating the base with 2,6-dichlorobenzyl bromide gave 70% *N*-(2,6-dichlorobenzyl)-4-(4-phenyl-2-thiazolyl)pyridinium bromide, decomp. 250–52° (MeOH), λ (log ε) 373 mμ (4.11), 265 mμ (4.30) (H_2O). Desyl chloride and III gave 10% 4-(4,5-diphenyl-2-thiazolyl)pyridine, m. 163–4° (EtOH), λ (log ε) 336 mμ (4.16) (0.01*M* glycine buffer, pH 9.0, with 50% MeOH). The base and 2,6-dichlorobenzyl bromide gave 85% *N*-(2,6-dichlorobenzyl)-4-(4,5-diphenyl-2-thiazolyl)pyridinium bromide, decompg. 240–1° (MeOH), λ (log ε) 398 mμ (4.30) 273 mμ (4.15) (50% MeOH). Also prepd. were: *N*-(2,6-dichlorobenzyl)-4-(2-benzylthiazolyl)pyridinium bromide, decompg. 245–6° (EtOH), 80% yield, λ (log ε) 345 mμ (4.32) 283 mμ (3.71) 262 mμ (3.19) (H_2O); *N*-(2,6-dichlorobenzyl)-4-carboxypyridinium bromide, decompg. 222° (MeOH), 81% yield; *N*-(2,6-dichlorobenzyl)-4-carbomethoxypyridinium bromide, decompg. 172–4° (MeOH, pptd. by Et_2O), 92% yield; *N*-(2,6-dichlorobenzyl)-4-carbamoylpyridinium bromide, decompg. 263–5° (MeOH), λ (log ε) 265 mμ (3.76) (H_2O) [after redn. with $Na_2S_2O_4$, the 1,4(?)-dihydropyridine, m. 160–70° (MeOH), about 60% yield, λ (log ε) 218 mμ (4.23), 295 mμ (3.30) (MeOH); after redn. with $NaBH_4$, the 1,6(?)-dihydropyridine, decompg. 162–8° (EtOH), 82% yield, λ (log ε) 340 mμ (2.30) (MeOH)]. XVI. A third type of dihydropyridine isomer of nicotinamide. Kurt Wallenfels and Hans Schüly. *Ibid.* 215–21.—With H_2S, malonic acid dinitrile was converted to cyanothioacetamide which was condensed with acetylacetone to 2,4-dimethyl-5-cyano-6-mercaptopyridine. Methylation with Me_2SO_4 and treatment with Zn gave 2,4-dimethyl-5-cyanopyridine which on treatment with NH_3 and H_2O_2 in acetone gave 90% 4,6-dimethylnicotinamide (I), m. 164–5°. After refluxing 7.5 g. I with 12 g. 2,6-dichlorobenzyl bromide in 50 ml. MeOH 2 hrs. and cooling, 200 ml. Et_2O was added in small portions. After 6 hrs. the mixt. was filtered to give 18 g. *N*¹-(2,6-dichlorobenzyl)-4,6-dimethylnicotinamide bromide (II), m. 236–8° (decompn.) (H_2O). This hygroscopic material crystd. with 2 moles H_2O. After 14 hrs. drying *in vacuo* at 65° over P_2O_5, only 1 mole H_2O was present. Redn. of II with $Na_2S_2O_4$ in Na_2CO_3 gave 50–60% cryst. product, m. above 150° (MeOH), λ (ε in cc./mmole) 392 mμ (4690). In neutral soln. $AgNO_3$ was reduced instantly. Reduction with $NaBH_4$ and Na_2CO_3 gave 96% cryst. product with properties identical to those of the $Na_2S_2O_4$ redn. product. Comparison of the absorption spectra of this compd. with previously prepd. reduction products (cf. part XI) indicated that this compd. was a 1,2-dihydropyridine.

Frances L. Estes

The mechanism of hydrogen transfer with pyridine nucleotides. XVII. Model studies of the chemical nature of the activated hydrogen. Kurt Wallenfels and Manfred Gellrich (Univ. Freiburg, Ger.). *Chem. Ber.* 92, 1408–15 (1959); cf. preceding abstr.—By the action of electron donors upon the oxidized form (I) of diphosphopyridine-nucleotide models, dimerized reaction products were obtained. The possibility of the reducing dimerization of the diphosphopyridinenucleotide in the living cell as well as the significance of such a reaction for the mechanism of the biol. oxidn. were discussed. 1-Benzyl-3-aminoformylpyridinium chloride (II) (5 g.) in 200 cc. H_2O freed from O by bubbling with N, simultaneously a soln. of 12 g. $CrCl_3 \cdot 6H_2O$ reduced with Zn and 24 cc. 6*N* HCl and then treated with 100 cc. concd. NH_4OH, the resulting $CrCl_3$ soln. pressed with stirring into the soln. of II, the mixt. filtered after 0.5 hr., the residue washed with hot MeOH, and the MeOH washing evapd. yielded 2.25 g. 2,2′-bi(5-aminoformyl-1-benzyl-1,2-dihydropyridyl) (III), decompg. 191–3°. II (40 g.) in 800 cc. H_2O treated with 70 g. NH_4Cl, and 20–30 cc. NH_4OH, the mixt. treated with stirring with 40 g. Mg in portions of 6–8 g. during 5 hrs., cooled, the solid product washed with MeOH, recrystd. from EtOH yielded 7 g. III. Zn dust (12 g.) in 20 cc. H_2O treated slowly with stirring with 4 g. $CuSO_4$ in 40 cc. H_2O, dild. with 20 cc. concd. NH_4OH and 100 cc. MeOH, poured with stirring into 10 g. II in 40 cc. H_2O, stirred 20 min., filtered, the residue extd. under N 4 times with 40-cc. portions hot EtOH, the ext. concd. *in vacuo* at 40–50° and cooled several hrs. to −15°, and the mixt. filtered gave 1.5 g. III; 0.7 g. 2nd crop. 1-(2,6-Dichlorobenzyl)-3-(aminoformyl)pyridinium bromide (IV) (3.6 g.) reduced in the usual manner with $CrCl_3$ yielded 0.23 g. 2,2′-bi[5-aminoformyl-1-(2,6-dichlorobenzyl)-1,2-dihydropyridyl] (V), decomp. 179–82°. The reduction of 10 g. IV with Mg gave 0.7 g. V. 1-Propyl-3-(aminoformyl)pyridinium bromide (7.5 g.) in 100 cc. H_2O reduced in the usual manner with 9 g. Zn dust in 20 cc. H_2O (pretreated with 3 g. $CuSO_4$ in 30 cc. H_2O and 20 cc. concd. NH_4OH), the mixt. stirred 15 min., and the product isolated with hot EtOH gave 0.7 g. 2,2′-bi(5-aminoformyl-1-propyl-1,2-dihydropyridyl) (VI), yellow needles, decompg. 188–96° (inserted at 150°). III (1.5 g.) in 100 cc. EtOH hydrogenated 12 hrs. under ambient conditions over 2.5 g. Raney Ni, filtered, concd., dild. with 2 vols. Me_2CO, and the ppt. recrystd. from 200 cc. 30% MeOH gave 0.5 g. bipiperidyl analog (VII) of III, needles, m. 203–5°. 1-Benzyl-1,4-dihydronicotinamide (1.07 g.) in 150 cc. EtOH hydrogenated 0.5 hr. over 75 mg. PtO_2 gave 0.8 g. 1-benzyl-3-(aminoformyl)-piperidine, needles, m. 122–3° (H_2O). Methylene blue-$ZnCl_2$ double salt (160 mg.) in 50 cc. H_2O treated under N with 213 mg. III in 25 cc. CH_2Cl_2 and 15 cc. EtOH, the mixt. treated 3 hrs. with stirring with a stream of N and extd. continuously 3 hrs. with 75 cc. boiling CH_2Cl_2, the aq. phase boiled with C and evapd. *in vacuo*, and the residue recrystd. from 20 cc. EtOH gave 180 mg. II, prisms, decompg. 230–5°. V (155 mg.) treated in the same manner 3 days with 160 mg. methylene blue gave the pyridinium salt which was reduced with $Na_2S_2O_4$ to 42 mg. 1-(2,6-dichlorobenzyl)-1,4-dihydronicotinamide (VIII). The 1,6-dihydro isomer (IX) of VIII treated in the same manner as V gave 68 mg. VIII. II reduced with $Na_2S_2O_4$ yielded 1-benzyl-1,4-dihydronicotinamide, m. 121–2°. A comparative study of the reoxidation of reduced pyridine derivs. with 2,6-dichlorophenol-indophenol at pH 7 and 25°, with malachite green in EtOH at 25°, and with viologen in refluxing EtOH was carried out (substrate, 2nd-order rate const., k_2 l./mole/min., of the reduction of 2,6-dichlorophenol-indophenol, and qualitative result of the reductions of malachite green and viologen given): VIII, 220, fast, no reaction; IX, 190, very slow, very slow; 2,4-di-Me deriv. of IX, rapid, very slow, slow; III, 20000, no reaction, fast. The ultraviolet absorption spectra of VIII, IX, the 1,2-isomer of IX, III, V, and VI were recorded.

F. W. Hoffmann

Pyridine analogs of tetrahydropteroic acid. Roy C. DeSelms (Stanford Univ., Stanford, Calif.). *Univ. Microfilms* (Ann Arbor, Mich.), *L.C. Card* No. Mic 59-3693, 89 pp.; *Dissertation Abstr.* 20, 1164–5(1959). P. M. B.

Phosphorylation. III. Synthesis of pyridoxine 5-phosphate via the phosphite. Teruo Tanaka (Toa Alimentary Chem. Inds., Ltd.). *Yakugaku Zasshi* 79, 1301–5(1959); cf. *C.A.* 53, 21988*d*.—A mixt. of 5 g. pyridoxine-HCl, 10 g. PhCHO, and 5 g. $ZnCl_2$ stirred 3 days at 50°, 50 ml. 10% Na_2CO_3 added, the ppt. filtered off, and the filtrate extd. with $CHCl_3$ gave 3.7 g. benzylidenepyridoxine (I), m. 151° (C_6H_6). I (2.6 g.) in 1.5 ml. Et_3N and 20 ml. $CHCl_3$ at 0° treated dropwise with 2.7 g. $(PhO)_2POCl$ in 10 ml. $CHCl_3$, kept 1 hr. at room temp., the $CHCl_3$ removed, the residue treated with CCl_4, the $Et_3N \cdot HCl$ filtered off, the filtrate concd., the residue heated 2 hrs. at 80° with 40 ml. 75%

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* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Crossover limits have been increased. See HELP CROSSOVER for details.

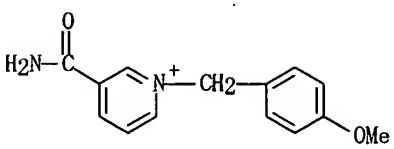
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d ide l8 tot

L8 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN **459165-10-7** REGISTRY
ED Entered STN: 04 Oct 2002
CN **Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, salt with trifluoromethanesulfonic acid (1:1) (9CI)** (CA INDEX NAME)
MF **C14 H15 N2 O2 . C F3 O3 S**
SR CA
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

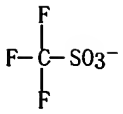
CM 1

CRN 175979-55-2
CMF C14 H15 N2 O2



CM 2

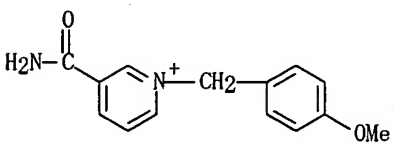
CRN 37181-39-8
CMF C F3 O3 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

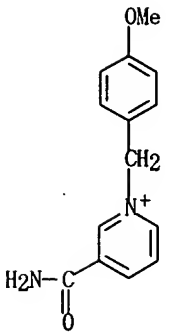
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN **175979-55-2** REGISTRY
ED Entered STN: 08 May 1996
CN **Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI)** (CA INDEX NAME)
FS 3D CONCORD
MF **C14 H15 N2 O2**
CI COM
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2005 ACS on STN
RN **63828-55-7** REGISTRY
ED Entered STN: 16 Nov 1984
CN **Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI)** (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN **3-Carbamoyl-1-(p-methoxybenzyl)pyridinium chloride (7CI)**
OTHER NAMES:
CN N-4'-Methoxybenzylnicotinamide chloride
MF **C14 H15 N2 O2 . Cl**
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)
CRN (175979-55-2)



● Cl⁻

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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(FILE 'HOME' ENTERED AT 13:32:22 ON 04 MAY 2005)

FILE 'REGISTRY' ENTERED AT 13:32:30 ON 04 MAY 2005
L1 177 SEA ABB=ON PLU=ON C14H15N2O2 AND NR=2 AND 46.150.18/RID
L2 QUE ABB=ON PLU=ON (PMS OR MAN OR IDS)/CI OR UNSPECIFIED OR COMPD OR COMPOUND OR (D OR T)/ELS
L3 169 SEA ABB=ON PLU=ON L1 NOT L2
L4 6 SEA ABB=ON PLU=ON L3 AND 3 (1A) CARBAMOYL?
L5 1 SEA ABB=ON PLU=ON L4 AND METHOXYPHENYL
D SCA
L6 49 SEA ABB=ON PLU=ON L3 AND METHOXYPHENYL
D STR TOT
SEL RN 19 30 44
L7 3 SEA ABB=ON PLU=ON (175979-55-2/BI OR 459165-10-7/BI OR 63828-55-7/BI) AND L6
D SCA
L8 3 SEA ABB=ON PLU=ON L5 OR L7

FILE 'HCAPLUS' ENTERED AT 13:43:00 ON 04 MAY 2005
L9 11 SEA ABB=ON PLU=ON L8 OR CARBAMOYL (2A) (METHOXYBENZYL OR METHOXY (1A) BENZYL) (1A) PYRIDIN? (1A) CHLORID?
E WAGLE D/AU
L10 123 SEA ABB=ON PLU=ON ("WAGLE D"/AU OR "WAGLE D G"/AU OR "WAGLE D R"/AU OR "WAGLE D S"/AU OR "WAGLE D T"/AU)
E WAGLE DILIP/AU
L11 58 SEA ABB=ON PLU=ON ("WAGLE DILIP"/AU OR "WAGLE DILIP R"/AU OR "WAGLE DILIP RAGHUNATH"/AU)
E GALL M/AU
L12 46 SEA ABB=ON PLU=ON ("GALL M"/AU OR "GALL M A"/AU OR "GALL M B"/AU OR "GALL M J"/AU OR "GALL M P"/AU)
E GALL MARTIN/AU
L13 83 SEA ABB=ON PLU=ON "GALL MARTIN"/AU
E BELL S/AU
L14 111 SEA ABB=ON PLU=ON ("BELL S"/AU OR "BELL S C"/AU)
E BELL STAN/AU
L15 242 SEA ABB=ON PLU=ON ("BELL STAN"/AU OR "BELL STANELY C"/AU OR "BELL STANLEY"/AU OR "BELL STANLEY C"/AU OR "BELL STANLEY CHARLES"/AU)
L16 1 SEA ABB=ON PLU=ON L9 AND (L10 OR L11 OR L12 OR L13 OR L14 OR L15)
L17 10 SEA ABB=ON PLU=ON L9 NOT L16
L18 QUE ABB=ON PLU=ON PY<=2000 OR AY<=2000 OR PRY<=2000
L19 9 SEA ABB=ON PLU=ON L17 AND L18

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     FILE 'HCAOLD' ENTERED AT 13:47:19 ON 04 MAY 2005
L20            1 SEA ABB=ON  PLU=ON  L8 OR CARBAMOYL (2A) (METHOXYBENZYL OR
                 METHOXY (1A) BENZYL) (1A) PYRIDIN? (1A) CHLORID?
                 D SCA
                 SEL AN
                 EDIT E1 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 13:47:53 ON 04 MAY 2005
L21            2 SEA ABB=ON  PLU=ON  "CA59:9970A"/OREF
L22            0 SEA ABB=ON  PLU=ON  L21 AND (L10 OR L11 OR L12 OR L13 OR L14
                 OR L15)
L23            2 SEA ABB=ON  PLU=ON  L21 AND L18
L24           10 SEA ABB=ON  PLU=ON  L19 OR L23

=> b hcap
FILE 'HCAPLUS' ENTERED AT 13:48:58 ON 04 MAY 2005
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FILE COVERS 1907 - 4 May 2005  VOL 142 ISS 19
FILE LAST UPDATED: 3 May 2005  (20050503/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> d all hitstr l16 tot

L16  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2002:675770  HCAPLUS
DN   137:216955
ED   Entered STN:  08 Sep 2002
TI   Method for treating fibrotic diseases or other indications using
     thiadiazolium, pyridinium and pyrimidinium salts
IN   Wagle, Dilip; Gall, Martin; Bell, Stanley C.
     ; Lavoie, Edmond J.
PA   Alteon, Inc., USA
SO   PCT Int. Appl., 104 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
IC   ICM  A61K
CC   28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
     Section cross-reference(s): 1
FAN. CNT 1
     PATENT NO.          KIND   DATE       APPLICATION NO.        DATE
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PI   WO 2002067851       A2     20020906   WO 2001-US49833        20011228
     WO 2002067851       A3     20030206
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
             RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ,
             VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW:  GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
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CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
CA 2433425 AA 20020906 CA 2001-2433425 20011228
EP 1355645 A2 20031029 EP 2001-273859 20011228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004525904 T2 20040826 JP 2002-567223 20011228
US 2002183365 A1 20021205 US 2001-36857 20011231
US 2004097495 A1 20040520 US 2003-691839 20031023
PRAI US 2000-259294P P 20001229
US 2001-259238P P 20010102
US 2001-296246P P 20010606
WO 2001-US49833 W 20011228
US 2001-36857 A1 20011231

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2002067851	ICM	A61K
JP 2004525904	FTERM	4C036/AD08; 4C036/AD21; 4C036/AD30; 4C055/AA06; 4C055/AA10; 4C055/BA01; 4C055/CA02; 4C055/CA34; 4C055/CB17; 4C055/DA01; 4C086/AA01; 4C086/AA02; 4C086/BC17; 4C086/BC86; 4C086/MA01; 4C086/MA04; 4C086/NA14; 4C086/ZA02; 4C086/ZA16; 4C086/ZA42; 4C086/ZA45; 4C086/ZA55; 4C086/ZA59; 4C086/ZA68; 4C086/ZA75; 4C086/ZA81; 4C086/ZA89; 4C086/ZA94; 4C086/ZA96; 4C086/ZB15; 4C086/ZB26; 4C086/ZB32; 4C086/ZC20
US 2002183365	NCL	514/341.000; 514/252.050; 514/255.050; 514/256.000; 514/242.000; 514/396.000; 514/406.000; 544/182.000; 544/238.000; 544/333.000
	ECLA	A61K031/4196; A61K031/433; A61K031/452; A61K031/505
US 2004097495	NCL	514/227.500; 514/383.000; 514/396.000; 514/406.000; 514/231.200; 514/252.100; 514/315.000; 514/365.000; 514/374.000; 514/242.000
	ECLA	A61K031/4196; A61K031/433; A61K031/452; A61K031/505; C07D213/82D; C07D239/26B; C07D285/12D6B; C07D521/00B1E2B

OS MARPAT 137:216955

AB The title compds. YAr+X- [I; Ar = 5-6 membered heteroaryl ring having a first ring N atom and optionally second or third ring N atoms, with the remaining ring atoms being C, O, or S, (provided the first N atom of Ar is a quaternary N and Ar is not thiazolium, oxazolium or imidazolium); Y is substituted on the first ring N atom (with the proviso that if Ar is pyrazole, indazole, triazole, benzotriazole, the second ring N atom is substituted with alkyl, alkoxycarbonylalkylene, aryl, etc.); Ar can be substituted on ring C atoms with aryl, carbamoyl, aralkyl, etc.; Y = CHR5R6 (R5 = H, alkyl, cycloalkyl, etc.; R6 = H, alkyl, alkenyl, etc.); X = a pharmaceutically acceptable anion, which may be absent if the compound provides a neutralizing salt], useful in treating or ameliorating certain fibrotic diseases or other indications linked to or associated with the formation of excess collagen, in an animal, including a human, were prepared Thus, refluxing 2-aminothiadiazole with 2-bromoacetamide in MeCN for 5 h afforded 5-amino-3-carbamoylmethyl-[1,3,4]thiadiazolium bromide. Assays to determine the activity of compds. I in breaking, reversing or inhibiting the formation of advanced glycosylation end products (AGEs) or AGE-mediated cross-links was presented (no data).

ST thiadiazolium pyridinium pyrimidinium salt prepn advanced glycosylation endproduct AGE; fibrosis thiadiazolium pyridinium pyrimidinium salt prepn

IT Glycoproteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(AGE (advanced glycosylation end product); preparation of thiadiazolium, pyridinium and pyrimidinium salts for reversing advanced glycosylation cross-links)

IT Inflammation
(Crohn's disease, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Intestine, disease
(Crohn's, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT Artery, disease

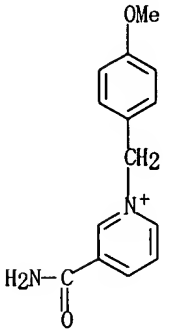
Inflammation
(arteritis, treatment of temporal; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Prostate gland, disease
(benign hyperplasia, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Hyperplasia
(benign prostatic, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Fibrosis
(cutaneous, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Mammary gland, disease
(fibrocystic, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Liver, disease
Lung, disease
Skin, disease
(fibrosis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Fibrosis
(hepatic, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Muscle, disease
(hypertrophy, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Intestine, disease
(inflammatory, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Connective tissue, disease
(mixed connective tissue disease, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Hypertrophy
(muscular, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Artery, disease
Inflammation
(periarteritis nodosa, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Pleura, disease
(pleurisy, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Anti-inflammatory agents
Human
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Fibrosis
(pulmonary, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Connective tissue, disease
(scleroderma, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Nervous system, disease
(sclerosis, treatment of cerebrosclerosis, annular sclerosis, diffuse sclerosis and lobar sclerosis; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Cystic fibrosis
Fibrosis
Hypertrophy
Myositis
Sarcoidosis
(treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT Blood vessel, disease
Inflammation
(vasculitis, treatment of; preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)
IT 13076-43-2P **63828-55-7P** 454704-85-9P 454704-86-0P
454704-87-1P 454704-88-2P 454704-89-3P 454704-90-6P 454704-91-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT 98-92-0, Nicotinamide 100-39-0, Benzyl bromide 104-83-6, 4-Chlorobenzyl chloride 289-95-2, Pyrimidine 456-04-2 459-46-1, 4-Fluorobenzyl bromide 589-17-3, 4-Bromobenzyl chloride 683-57-8, 2-Bromoacetamide 824-94-2, 4-Methoxybenzyl chloride 937-20-2, 2-Chloro-1-(4-chlorophenyl)ethanone 4005-51-0, 2-Aminothiadiazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

IT **63828-55-7P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of thiadiazolium, pyridinium and pyrimidinium salts for treating fibrotic diseases)

RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



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L24 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:619241 HCAPLUS
DN 125:300276
ED Entered STN: 18 Oct 1996
TI Reactions of Charged Substrates. 5. The Solvolysis and Sodium Azide Substitution Reactions of Benzylpyridinium Ions in Deuterium Oxide
AU Buckley, Neil; Oppenheimer, Norman J.
CS Department of Pharmaceutical Chemistry, University of California, San Francisco, CA, 94143-0446, USA
SO Journal of Organic Chemistry (**1996**), 61(21), 7360-7372
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 7
AB Second-order rate consts. and activation values were measured for the reactions with NaN3 of a series of 4-Y-substituted (Y = MeO, Me, H, Cl, and NO2) benzyl 3'-Z-substituted (Z = CN, CONH2, H, F, Ac) pyridinium chlorides in deuterium oxide. 3'-Cyanopyridine substrates reacted much faster than nicotinamide and pyridine substrates; in the pyridine series the 4-Me, 4-H, and 4-Cl benzyl analogs did not react for up to 6 mo at 96° in 1.7 M NaN3. The 3'-cyanopyridine substrates do not exhibit

borderline kinetic behavior, but the nicotinamide substrates do. The Hammett plot is flat for the NaN3 reaction of 3'-cyanopyridine substrates and increasingly V-shaped for the nicotinamide and pyridine substrates. The values of βLG (four-point plot) for the NaN3 reaction of the 4-MeO benzyl substrates is -1.45, which is usually interpreted as being a very "late" activated complex. Two-point Bronsted "plots" for the other benzyl derivs. and for two N-methylpyridinium ions give values of βLG in the same range. The second-order rate constant and activation values for N-methyl-3'-cyanopyridinium iodide are within the same range as those for the benzyl substrates. For the hydrolysis reaction, the Hammett plot is linear for 3'-cyanopyridine substrates ($\rho+ = -1.24$) and flat for the nicotinamide substrates. The extent of hydrolysis of 0.005-0.05 M solns. of the 3'-cyanopyridinie substrates depended on the initial concentration of substrate, and hydrolysis was slowed significantly or stopped completely in the presence of exogenous 3-cyanopyridine. These results show that an equilibrium is established among the products for the 4-MeO, 4-Me, 4-H, and 4-Cl substrates; the 4-NO2 substrate reacted too slowly to discern any difference. Data for the extent of hydrolysis were fitted by an equation derived assuming the equilibrium Despite this limitation on a classic test of mechanism, the rates and ρ values are consistent with direct displacement by solvent and not with a unimol. process. These results, which are rationalized in terms of the Pross-Shaik model, suggest that there are no ion-dipole complex intermediates in the benzyl series and show that borderline kinetic behavior is a function of leaving group ability and is not necessarily related to a change in mechanism. A computational approach was used to evaluate anomalous βLG values for the hydrolysis and nucleophilic substitution reactions of the methylpyridinium ion substrates. It was found that neither the Nu-substrate bond lengths nor the difference in charge matched the βLG values. The value of ΔΔS. thermod. of -15 gibbs/mol . between (4-methoxybenzyl)-3'-cyanopyridinium chloride and the corresponding dimethylsulfonium chloride in the NaN3 reaction, which is the result of the solvation of the pyridine at the transition state and the lack of solvation of SMe2, is used to argue that the source of NAD+ glycohydrolase "catalysis" of NAD+ bond cleavage is the result of desolvation of the leaving group upon binding.

ST benzylpyridinium hydrolysis azide substitution kinetics mechanism; reaction const benzylpyridinium hydrolysis azide substitution; NAD glycohydrolase catalysis

IT Electron configuration and Electron density
Heat of hydrolysis
Hydrolysis
Kinetics of hydrolysis
Leaving group effects
Linear free energy relationship
Potential energy surface and hypersurface
Reaction constant
Substituent effect
Substitution reaction, nucleophilic
Transition state structure
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Pyridinium compounds
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Molecular orbital
(frontier, kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT Heat of substitution reaction
Kinetics of substitution reaction
(nucleophilic, kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT 2876-13-3
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(estimated; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

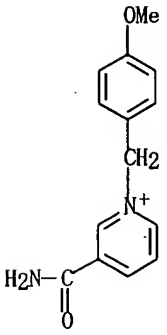
IT 594-09-2, Trimethylphosphine 1004-16-6, 3-Cyano-1-methylpyridinium

iodide 4329-72-0 5096-13-9 6456-44-6 6621-73-4 6951-52-6
14343-69-2, Azide 14535-08-1 14535-12-7 20461-54-5, Iodide,
reactions 26628-22-8, Sodium azide 52354-19-5 **63828-55-7**
74796-72-8 76053-06-0 87976-56-5 98349-72-5 183054-49-1
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT 7732-18-5, Water, reactions 15923-33-8 183054-50-4
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(potential surface calcn.; kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

IT **63828-55-7**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of solvolysis and sodium azide substitution reactions of benzylpyridinium ions)

RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L24 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:191937 HCAPLUS
DN 124:316412
ED Entered STN: 04 Apr 1996
TI Reactions of Charged Substrates. 4. The Gas-Phase Dissociation of (4-Substituted benzyl)dimethylsulfoniums and -pyridiniums
AU Buckley, Neil; Maltby, David; Burlingame, Alma L.; Oppenheimer, Norman J.
CS School of Pharmacy, University of California, San Francisco, CA, 94143-0446, USA
SO Journal of Organic Chemistry (**1996**), 61(8), 2753-62
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
CC 22-12 (Physical Organic Chemistry)
Section cross-reference(s): 33
AB The relative rates for the gas-phase dissociation RX+ → R+ + X° of five (4-Y-substituted benzyl)dimethysulfoniums (Y = MeO, Me, H, Cl, and NO2) and 24 (4-Y-substituted benzyl)-3'-Z-pyridiniums (complete series for Z = CN, Cl, CONH2, and H, and 4-methoxy- and 4-nitrobenzyls for Z = F and CH3CO) were measured using liquid secondary ion mass spectrometry. The Hammett plot (vs δΔG0 or σ+) is linear for the sulfoniums, but plots for the four pyridinium series have a drastic break between the 4-Cl and 4-NO2 substrates. Broensted-like plots for the pyridiniums show a strong leaving group effect only for 4-nitrobenzyls. An anal. of these linear free energy relations with supporting evidence from semiempirical computations suggests that collisionally activated

pyridinium substrates dissociate through two pathways, direct dissociation and an ion-neutral complex intermediate. Comparison of these results with results for the solution reactions of some of these compds. shows that the mechanism is different in the gas and solution phases. Sufficient exptl. data are not available to assign a mechanism for dissociation to the sulfonium series, but computational results show characteristics of a direct dissociative mechanism.

ST dissocn gas phase benzyldimethylsulfonium benzyldimethylpyridinium; sulfonium benzyldimethyl gas phase dissocn; pyridinium benzyldimethyl gas phase dissocn

IT Linear free energy relationship
Reaction constant
(for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT Dissociation
Kinetics of dissociation
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT Leaving group effects
Substituent effect
(on gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

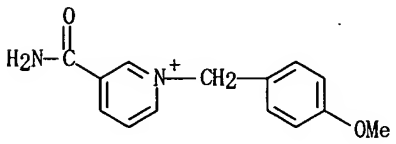
IT Linear free energy relationship
(Broensted, for gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT 15519-25-2 16183-83-8 16183-87-2 24837-70-5 38332-27-3
45809-04-9 45964-81-6 46122-80-9 46441-13-8 48120-95-2
58219-38-8 58219-39-9 71897-24-0 71897-27-3 78186-22-8
133227-04-0 **175979-55-2** 175979-56-3 175979-57-4
175979-58-5 175979-59-6 175979-60-9 175979-61-0 175979-62-1
175979-63-2 175979-64-3 175979-65-4 175979-66-5 175979-67-6
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

IT **175979-55-2**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetics and mechanism of gas-phase dissociation of substituted benzyldimethylsulfoniums and -pyridiniums)

RN 175979-55-2 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



L24 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1990:422794 HCAPLUS

DN 113:22794

ED Entered STN: 21 Jul 1990

TI Addition of cyanide ion to nicotinamide cations in acetonitrile. Formation of nonproductive charge-transfer complexes

AU Engbersen, Johan F. J.; Koudijs, Arie; Sleiderink, Hedwig M.; Franssen, Maurice C. R.

CS Lab. Org. Chem., Agric. Univ., Wageningen, 6703 HB, Neth.

SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (**1990**), (1), 79-83
CODEN: JCPKBH; ISSN: 0300-9580

DT Journal

LA English

CC 22-4 (Physical Organic Chemistry)

OS CASREACT 113:22794

AB The mixing of equal vols. of 0.2 mmol dm-3 1-benzylnicotinamide ion and 2 mmol dm-3 cyanide ion results in the immediate formation of a transient absorption band at 375 nm which can be ascribed to a charge-transfer complex. This complex disappears within ca. 0.2 s with the formation of the 1,6-addition product which, in turn, is rapidly converted into the thermodynamically more stable 1,4-adduct. Me substitution at the 6-position of the nicotinamide ring inhibits the formation of the 1,6-adduct, resulting in an increase in the lifetime of the charge-transfer complex. Subsequently a mixture of the 1,4-cyanide adduct and, most likely, the 1,2-adduct is formed. Rate effects with variation of substituents in the 1-benzyl group reveal that charge-transfer complex formation is counterproductive to the formation of addition products.

ST cyanide ion addn nicotinamide cation; charge transfer complex cyanide nicotinamide; substituent effect cyanide addn nicotinamide

IT Reaction constant
(for addition, dissociation, and charge-transfer-complexation processes in cyanide ion-nicotinamide cation systems)

IT Addition reaction
(of cyanide ion with nicotinamide cations, formation of nonproductive charge-transfer complexes in)

IT Kinetics of addition reaction
(of cyanide ion with nicotinamide cations, solvent and substituent effects on)

IT Kinetics of dissociation
(of cyanide-ion adducts with nicotinamide cations, solvent and substituent effects on)

IT Ultraviolet and visible spectra
(of transient species, in addition reaction of cyanide ion with nicotinamide cations)

IT Substituent effect
(on addition, dissociation, and charge-transfer-complexation processes in cyanide ion-nicotinamide cation systems)

IT 151-50-8, Potassium cyanide (K(CN))
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with nicotinamide cations)

IT 127678-22-2 127678-24-4 127678-25-5 127678-27-7 127678-29-9
RL: PROC (Process)
(decay of, kinetics of)

IT 13076-43-2P 54027-58-6P 63761-90-0P 63761-95-5P **63828-55-7P**
70293-11-7P 127663-01-8P 127663-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with cyanide)

IT 96551-72-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation and addition reaction of, with cyanide)

IT 127663-05-2P 127663-06-3P 127663-07-4P 127678-20-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and charge-transfer complexation of, with cyanide)

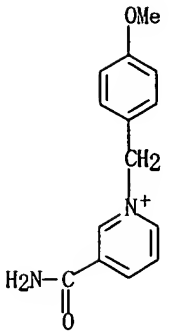
IT 19432-61-2P 75420-69-8P 75420-70-1P 75420-71-2P 75420-74-5P
127663-03-0P 127663-04-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and dissociation of, kinetics of)

IT 127663-08-5P 127663-09-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with cyanide)

RN 63828-55-7 HCAPLUS

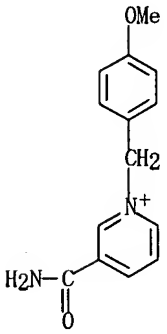
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl^-

L24 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:166806 HCAPLUS
DN 108:166806
ED Entered STN: 13 May 1988
TI Polarographic reduction of p-substituted 1-phenyl-3-(aminocarbonyl)pyridinium salts
AU Krechl, Jiri; Mizaninoiva, Daniela; Volke, Jiri; Kuthan, Josef
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28, Czech.
SO Collection of Czechoslovak Chemical Communications (**1987**), 52(6), 1550-60
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 72
AB The substituent effect (H, NO2, CO2H, Br, Cl, NHAc, Me, OMe, OH, NEt2) on the polarog. behavior of p-substituted 1-phenyl-3-aminocarbonylpyridinium cations has been investigated, in particular on their half-wave potentials in aqueous phosphate buffers pH 6·65 (10% DMF) and in anhydrous solns. of DMF with 0·05 mol L-1 Bu4N+ BF4- as supporting electrolyte. The half-wave potentials of the reduction wave which corresponds to the uptake of a single electron (wave B) and to the formation of the primary radical, obey a Hammett correlation in a way similar to the case of 1-benzyl-3-aminocarbonylpyridinium cations. The slope Qπ,R in the Hammett plot equals 0·093 V for 10% DMF and 0·179 V for anhydrous DMF and compares thus with the slope obtained with the 1-benzyl derivs. where 0.05 V was found for water and 0·127 V of anhydrous acetonitrile. The transfer of the substituent effect from the substituent in the para position on the benzene nucleus to the heterocyclic ring is thus equally active in both substances and depends more strongly on the solvent than on the structure of the cation of both types. The low sensitivity in both series towards a change in the substituent is explained by the fact that during the uptake of the electron the benzene and the pyridine nucleus are not even approx. coplanar. This is why the π-overlap between the two nuclei is considerably restricted. The anal. of sampled d.c.-polarog. waves has confirmed that the one-electron uptake is followed by a chemical reaction, most probably a dimer formation or a reaction of the primary product with the starting substance.
ST polarog redn pyridinium salt; amidopyridinium phenyl electrochem redn LFER
IT Reduction
(of substituted phenyl(aminocarbonyl)pyridinium salts, substituent effects on)
IT Substituent effect
(on polarog. reduction of phenyl(aminocarbonyl)pyridinium salts)
IT 5096-13-9 6951-52-6 52354-19-5 **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)
IT 54027-59-7P 54027-60-0P 69986-64-7P 76911-53-0P 76911-55-2P
76911-56-3P 87384-49-4P 87384-51-8P 87384-52-9P 112445-86-0P

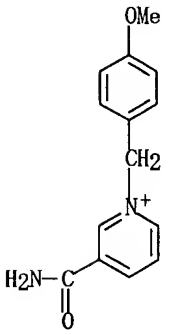
113849-47-1P 113849-48-2P 113849-49-3P 113849-50-6P 113849-53-9P
113849-54-0P 113849-55-1P 113849-57-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and polarog. reduction of)
IT 98-92-0, Nicotinamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with anilines)
IT 62-53-3, reactions 93-05-0 100-01-6, reactions 104-94-9, 4-Methoxyaniline 106-40-1, 4-Bromoaniline 106-47-8, 4-Chloroaniline, reactions 106-49-0, reactions 122-80-5, 4-Acetamidoaniline 123-30-8, 4-Hydroxyaniline 150-13-0, 4-Aminobenzoic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nicotinamide)
IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(polarog. reduction of)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L24 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1985:422428 HCAPLUS
DN 103:22428
ED Entered STN: 27 Jul 1985
TI Selective reduction of pyridinium, quinolinium, and pyrazinium salts to the dihydro stage with 1-benzyl-1,2-dihydroisonicotinamide
AU Nuvole, Antonio; Paglietti, Giuseppe; Sanna, Paolo; Acheson, R. Morrin
CS Ist. Chim. Farm., Univ. Sassari, Sassari, 07100, Italy
SO Journal of Chemical Research, Synopses (**1984**), (11), 356-7
CODEN: JRPSDC; ISSN: 0308-2342
DT Journal
LA English
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 22, 28
OS CASREACT 103:22428
AB Quinolinium, pyridinium, and pyrazinium salts were reduced selectively to 1,4-dihydroquinolines, 1,4-dihydropyridines, and 1,6-dihydropyrazines, resp., by 1-benzyl-1,2-dihydroisonicotinamide (I) in dry MeOH under N. E.g., reduction of N-benzyl-3-carbamoylquinolinium bromide by I for 5 min gave N-benzyl-1,4-dihydroquinoline-3-carboxamide quant.
ST benzylisonicotinamide redn quinolinium pyridinium pyrazolinium; isonicotinamide benzyl redn quaternary compd; regioselective redn quaternary compd benzylisonicotinamide; quinolinium redn benzylisonicotinamide regioselective; pyridinium redn benzylisonicotinamide regioselective; pyrazinium redn benzylisonicotinamide regioselective
IT Regiochemistry
(of reduction of quinolinium, pyridinium, or pyrazinium compds. by

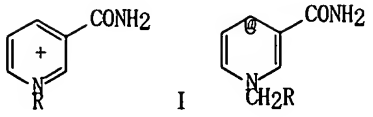
benzyldihydroisonicotinamide)
IT Reduction
(regioselective, of quinolinium, pyridinium, and pyrazinium compds. by benzyldihydroisonicotinamide)
IT 62417-98-5P 96421-80-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and selective reduction of, by benzyldihydroisonicotinamide)
IT 96421-81-7P 96421-82-8P 96421-83-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 952-92-1P 2288-38-2P 17260-79-6P 17750-23-1P 19350-64-2P
20224-92-4P 34865-02-6P 37589-77-8P 56133-30-3P 57355-62-1P
71127-33-8P 73027-91-5P 74124-15-5P 78224-91-6P 88928-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by selective reduction of quaternary compound with benzyldihydroisonicotinamide)
IT 100-39-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization by, of Me quinolinecarboxylate, cyanopyridine, and pyrazinecarboxamide)
IT 98-96-4 100-48-1 53951-84-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(quaternization of, by benzyl bromide)
IT 75532-98-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction by, of quinolinium, pyridinium, and pyrazinium compds., regioselective)
IT 5496-66-2 6456-44-6 6516-41-2 6516-53-6 13076-43-2 13958-90-2
26368-94-5 **63828-55-7** 70293-11-7 73027-90-4 96421-79-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by benzyldihydroisonicotinamide, regioselective)
IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by benzyldihydroisonicotinamide, regioselective)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

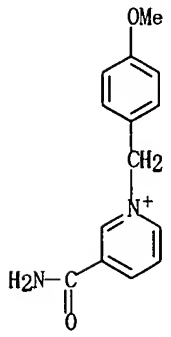
L24 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:504507 HCAPLUS
DN 99:104507
ED Entered STN: 12 May 1984
TI Dihydropyridines. XLVIII. Substituent effect in addition of cyanide ion to p-substituted 1-benzyl-3-carbamoylpyridinium chlorides
AU Pavlikova-Raclova, Frantiska; Kuthan, Josef
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (**1983**), 48(5), 1401-7

CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 22-4 (Physical Organic Chemistry)
GI



I II

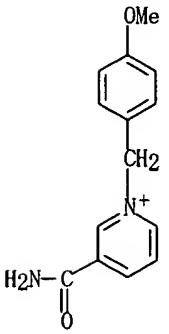
AB Rate consts. for the title reaction were determined in aqueous solns. of 8 quaternary salts of nicotinamide (I; R = p-XC6H4CH2; X = MeO, Me, H, F, Cl, CO2Me, cyano, NO2). Good Hammett correlations were found, along with correlation of E1/2 of polarog. reduction of I with rate and equilibrium consts. In aqueous media, reduction of I (same R; X = Me, H, F, Cl, MeO) with π-donor substituents proceeds via a simple E mechanism I → II, whereas in the case of π-acceptor substituents (I; X = NO2, CN, CO2Me), radicals II are formed via a 3-step CEC mechanism.
ST cyanation benzylcarbamoylpyridinium kinetics mechanism; LFER cyanation benzylcarboamoylpyridinium
IT Linear free energy relationship
(in cyanation of benzylcarbomoylpyridinium chlorides)
IT Cyanation
(of benzylcarbamoylpyridinium chlorides, mechanism of)
IT Kinetics of cyanation
Reduction, electrochemical
(of benzylcarbomoylpyridinium chlorides)
IT 1652-58-0 5096-13-9 6621-73-4 6951-52-6 52354-19-5
63828-55-7 84354-35-8 84389-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of, kinetics and mechanism of)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L24 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:61940 HCAPLUS
DN 98:61940
ED Entered STN: 12 May 1984
TI Polarographic reduction of p-substituted 1-benzyl-3-carbamoylpyridinium chlorides

AU Kuthan, Josef; Pavlikova-Raclova, Frantiska
CS Dep. Org. Chem., Prague Inst. Chem. Technol., Prague, 166 28/6, Czech.
SO Collection of Czechoslovak Chemical Communications (**1982**), 47(11), 2890-903
CODEN: CCCCAK; ISSN: 0366-547X
DT Journal
LA English
CC 72-2 (Electrochemistry)
AB Substituent effects (H, NO2, CN, CO2Me, Me, MeO, Me2N, Cl, F) on polarog. characteristics of the title quaternary salts were studied in H2O, anhydrous MeCN, and aqueous EtOH. In the last solvent, 1 of the polarog. waves gradually disappears. The probable course of the investigated electrode processes and accompanying chemical transformations is discussed.
ST polarog redn benzyl carbamoylpyridinium chloride; quaternary nicotinamide chloride polarog redn
IT Substituent effect
(in polarog. reduction of benzylcarbamoylpyridinium chlorides)
IT Reduction, electrochemical
(of benzylcarbamoylpyridinium chloride p-substituted derivs.)
IT 1652-58-0 5096-13-9 6621-73-4 6951-52-6 52354-19-5
63828-55-7 84354-35-8 84389-20-8 84389-21-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)
IT **63828-55-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, electrochem.)
RN 63828-55-7 HCAPLUS
CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



● Cl⁻

L24 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1977:480366 HCAPLUS
DN 87:80366
ED Entered STN: 12 May 1984
TI Model dehydrogenase reactions. Catalysis of dihydronicotinamide reductions by noncovalent interactions
AU Hajdu, Joseph; Sigman, David S.
CS Sch. Med., Univ. California, Los Angeles, CA, USA
SO Biochemistry (**1977**), 16(13), 2841-6
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
CC 7-4 (Enzymes)
AB Carboxylate, pyrophosphate, and hydroxyl groups can accelerate the nonenzymic rates of dihydronicotinamide redns. via intramol. noncovalent interactions. The accelerations by the neg. charged carboxylate and pyrophosphate groups occur in nonpolar solvents but the effect of the hydroxyl groups occurs both in aqueous and nonaq. solution The largest effects are observed for neighboring carboxylate groups in nonpolar solvents; e.g.,

the 2nd-order rate constant for the reduction of N-methylacridinium ion by N-cis-2'-carboxycyclopentyldihydronicotinamide in acetonitrile is 1000-fold more rapid than the rate constant for the corresponding Me ester. Apparently, the neg. charged carboxylate stabilizes the partial pos. charge which develops on the nicotinamide moiety in the transition state. The conclusion that the neg. charged pyrophosphate can enhance dihydronicotinamide redns. is based on the observation that β-NADH reduces N-methylacridinium ion 30-fold faster in MeOH than in aqueous solution, whereas α-NADH reduces the oxidant only 7-fold faster in MeOH than in water. The pyrophosphate group enhances the reaction rates of both anomers by a distance-dependent field effect. The magnitude is greater for the β anomer because the pyrophosphate and nicotinamide moieties are nearer neighbors in this anomer. The rate accelerations produced by hydroxyl groups of alcs. are not as great as those observed for carboxylate groups in nonpolar solvents. In aqueous solns., α-NADH reduces 3 different oxidants 10-fold more rapidly than β-NADH. In acetonitrile, synthetic dihydronicotinamides containing hydroxyl groups increase the rate 6-fold. These modest accelerations with the neutral hydroxyl groups emphasize the importance of a neg. charged group in order to achieve large enhancements in nonaq. solns.

ST dehydrogenase model dihydronicotinamide redn

IT Functional groups
(diphosphate, in dihydronicotinamide reduction of methylacridinium, dehydrogenase reaction mechanism in relation to)

IT Carboxyl group
Hydroxyl group
(in dihydronicotinamide reduction of methylacridinium, dehydrogenase reaction mechanism in relation to)

IT Kinetics of reduction
(of methylacridinium, by alkyldihydronicotinamide derivs.)

IT 58-68-4D, analogs 21104-13-2 56133-27-8 56133-28-9 56133-30-3 56133-31-4 56133-32-5 56133-33-6 63761-81-9 63761-82-0 63761-83-1 63761-84-2 63761-85-3 63761-86-4 63761-87-5 63761-88-6 63762-01-6 63762-02-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-methylacridinium reduction by, dehydrogenase reaction mechanism in relation to)

IT 17750-24-2
RL: PRP (Properties)
(UV spectra of, solvent effect on)

IT 63762-03-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(chloranil reduction by, dehydrogenase reaction mechanism in relation to)

IT 9035-82-9
RL: PRP (Properties)
(models for, N-alkyldihydronicotinamide as)

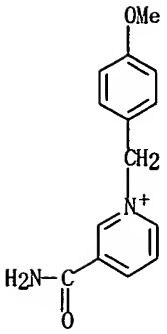
IT 5096-13-9P 7597-54-8P 63761-89-7P 63761-90-0P 63761-91-1P 63761-92-2P 63761-93-3P 63761-94-4P 63761-95-5P 63761-96-6P 63761-97-7P 63761-98-8P 63761-99-9P 63762-00-5P **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

IT 118-75-2, reactions 13367-81-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of, by dihydronicotinamide alkyl derivs., dehydrogenase reaction mechanism in relation to)

IT **63828-55-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



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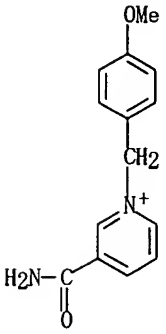
L24 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1963:454780 HCAPLUS
DN 59:54780
OREF 59:**9970a-c**
ED Entered STN: 22 Apr 2001
TI Action of base on quaternary salts of nicotinamide
AU Dittmer, Donald C.; Kolyer, J. M.
CS Univ. of Pennsylvania, Philadelphia
SO Journal of Organic Chemistry (**1963**), 28(9), 2288-94
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
CC 37 (Heterocyclic Compounds (One Hetero Atom))
GI For diagram(s), see printed CA Issue.
AB Treatment of 1benzyl-3-carbamoylpyridinium chloride with NaOH in dilute EtOH yielded a new substance (I), believed to be a cyclic trimer. The structure of I was based on its analysis, infrared spectrum, ultraviolet spectrum, fluorescence spectrum, proton magnetic resonance spectrum, mol. weight, and its chemical reactions. I is believed to have been formed by way of a pyridinium ylide. Several new pseudo base ethers of 1-substituted nicotinamide salts have been prepared
IT Spectra, visible and ultraviolet
(of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]-heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
IT Spectra, infrared
(of 1,6,11-triazatetracyclo[11.2.2.23.6.28.11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
IT Nuclear magnetic resonance
(of 1,6,11-triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide derivs.)
IT Bases
(reactions of, with 3-carbamoylpyridinium derivs.)
IT Nitrone, α-benzyl-N-[p-(dimethylamino)phenyl]-α-phenyl-
IT Pyridinium, 3-carbamoyl-
(derivs., reaction with bases)
IT 952-92-1, Nicotinamide, 1-benzyl-1,4-dihydro- 1652-58-0, Pyridinium, 3-carbamoyl-1-(p-fluorobenzyl)-, chloride 1893-57-8, Nicotinamide, 1-(p-fluorobenzyl)-1,4-dihydro- 2996-08-9, Nicotinamide, 4,4'-oxybis[1-(p-fluorobenzyl)-1,4-dihydro- 4533-64-6, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-fluorophenyl)- 5096-13-9, Pyridinium, 1-benzyl-3-carbamoyl-, chloride 6621-73-4, Pyridinium, 3-carbamoyl-1-(p-nitrobenzyl)-, chloride 6951-52-6, Pyridinium, 3-carbamoyl-1-(p-chlorobenzyl)-, chloride 13502-54-0, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,4-dihydro- 19355-18-1, Nicotinamide, 1-(2,6-dichlorobenzyl)-1,6-dihydro- **63828-55-7**, **Pyridinium**, 3-**carbamoyl**-1-(p-**methoxybenzyl**)-, **chloride** 75340-29-3, Nicotinamide, 4,4'-oxybis[1-benzyl-1,4-dihydro- 92578-90-0, Glycine, N-(p-tolylsulfonyl)-, 2-(p-

bromophenyl)hydrazide 93807-08-0, Glycine, N-(phenylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93946-35-1, Glycine, N-(p-tolylsulfonyl)-, 2-(m-bromophenyl)hydrazide 94379-06-3, Nipecotamide, 1-benzyl-, picrate 95945-13-4, Nicotinamide, 4,4'-oxybis[1,4-dihydro-1-(p-nitrobenzyl)- 96003-72-4, Nicotinamide, 4,4'-oxybis[1-(2,6-dichlorobenzyl)-1,4-dihydro- 96635-71-1, Nipecotamide, 1-benzyl-, hydrochloride 96650-48-5, Pyridinium, 3-carbamoyl-1-(2,4-dinitrobenzyl)-, chloride 98310-77-1, Pyridinium, 1-benzyl-3-carbamoyl-, oxalate 100210-41-1, Pyridinium, 1-benzyl-3-carbamoyl-, picrate 106141-61-1, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-bromophenyl)- 106141-62-2, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-chlorophenyl)- 106141-68-8, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-triphenyl- 106384-38-7, Pyridinium, 1-(p-bromobenzyl)-3-carbamoyl-, chloride
(preparation of)

IT **63828-55-7, Pyridinium, 3-carbamoyl-1-(p-methoxybenzyl)-, chloride**
(preparation of)

RN 63828-55-7 HCAPLUS

CN Pyridinium, 3-(aminocarbonyl)-1-[(4-methoxyphenyl)methyl]-, chloride (9CI) (CA INDEX NAME)



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L24 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1963:454779 HCAPLUS

DN 59:54779

OREF 59:**9969g-h, 9970a-c**

ED Entered STN: 22 Apr 2001

TI The reaction of cyanomethyl esters of carboxylic acids with arylhydrazines. III. Investigation of the influence of bromine substituents in the benzene ring of phenylhydrazine on the acylation reaction by cyanomethyl carboxylates

AU Grudzinska, P.

CS Univ. Lodz, Pol.

SO Lodz. Towarz. Nauk, Wydzial III, Acta Chim. (**1962**), 8, 131-40

DT Journal

LA English

CC 37 (Heterocyclic Compounds (One Hetero Atom))

GI For diagram(s), see printed CA Issue.

AB cf. CA 57, 16478i. oBrC6H4NHNH2.HCl, m. 184-5° (decomposition) (1:4 HCl-H2O), dissolved in hot H2O, basified with 3N KOH, and cooled yielded o-BrC6H4NHNH2 (I), needles, m. 46-8° . Similarly were prepared the m-isomer of I, straw-colored oil, b.-, 132-5D b20 174-6° , 53%, and the light yellow p-isomer of I, m. 105-77, 50% [HCl salt m. 201 3° (decomposition)]. The appropriate cyanomethyl ester (0.005 mole)4 and 0.006 mole of a suitable bromophenylhydrazine in 10 cc. EtOAc refluxed 9 (or 20 hrs.) yielded the corresponding RCONHNHC6H4Br (II); in this manner were prepared the following II (with o-Br)(R, % crude yield, and m.p. given):

BzNHCH2, 61, 184-5° (absolute EtOH) (71% during 20 hrs.); Ph-SO2NHCH2, 50, 130-1° (98% EtOH) (73% during 20 hrs.); pMeC6H4SO2NHCH2, 64.3, 121-3° (96% EtOH) (73.5% during 20 hrs.); 4-pyridyl, 27.4 (during 20 hrs.), 169-70° (EtOH). In the same manner were prepared the following II (with m-Br) (same data given): BzNHCH2, 88, 197 8° (EtOH); PhSO2-NHCH2, 84, 159 60° (EtOH); p-MeC6H4SO2NHCH2, 69.4, 154-5° (EtOH); 4-pyridyl, 48.5 (during 20 hrs.), - [HCl salt m. 261-3° (decomposition) (50% AcOH)]; and the following II (with p-Br) (same data given): BzNHCH2, 93, 213-15° (decomposition) (50% AcOH); PhSO2NHCH2, 100, 186-7° (decomposition) (96% EtOH); p-MeC6H4SO2NHCH2, 91, 195 6° (decomposition) (EtOH); 4-pyridyl, 42.5 (during 20 hrs.), - [HCl salt, yellow needles, m. 215° (decomposition) (aqueous HCl)].

IT Acylation
(by glycolonitrile esters)

IT Hydrazine, (m-bromophenyl)-
Nitrone, α-benzyl-N-[p-(dimethylamino)phenyl]-α-phenyl-

IT 302-01-2, Hydrazine
(aryl derivs., reaction with glycolonitrile esters)

IT 100-63-0, Hydrazine, phenyl-
(derivs., in acylation by glycolonitrile esters)

IT 110-94-1, Glutaric acid
(derivs., reaction with 3-(2-aminoethyl)indole)

IT 75-05-8, Acetonitrile
(esters)

IT 107-16-4, Glycolonitrile
(esters, reaction with arylhydrazines)

IT 7726-95-6, Bromine
(in acylation by glycolonitrile esters)

IT 589-21-9, Hydrazine, (p-bromophenyl)- 4533-64-6, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-fluorophenyl)- 16732-66-4, Hydrazine, (o-bromophenyl)- 50709-33-6, Hydrazine, (o-bromophenyl)-, hydrochloride 91912-33-3, Succinimide, N-[(dimethylamino)methyl]-, hydrochloride 92425-57-5, Hippuric acid, 2-(o-bromophenyl)hydrazide 92576-81-3, Isonicotinic acid, 2-(o-bromophenyl)hydrazide 92578-89-7, Glycine, N-(p-tolylsulfonyl)-, 2-(o-bromophenyl)hydrazide 92578-90-0, Glycine, N-(p-tolylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93807-06-8, Glycine, N-(phenylsulfonyl)-, 2-(m-bromophenyl)hydrazide 93807-07-9, Glycine, N-(phenylsulfonyl)-, 2-(o-bromophenyl)hydrazide 93807-08-0, Glycine, N-(phenylsulfonyl)-, 2-(p-bromophenyl)hydrazide 93897-68-8, Hippuric acid, 2-(m-bromophenyl)hydrazide 93897-69-9, Hippuric acid, 2-(p-bromophenyl)hydrazide 93946-35-1, Glycine, N-(p-tolylsulfonyl)-, 2-(m-bromophenyl)hydrazide 94379-06-3, Nipecotamide, 1-benzyl-, picrate 95592-93-1, Isonicotinic acid, 2-(m-bromophenyl)hydrazide, hydrochloride 95592-94-2, Isonicotinic acid, 2-(p-bromophenyl)hydrazide, hydrochloride 96635-71-1, Nipecotamide, 1-benzyl-, hydrochloride 106141-61-1, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-bromophenyl)- 106141-62-2, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-tris(p-chlorophenyl)- 106141-68-8, 1,6,11-Triazatetracyclo[11.2.2.23,6.28,11]heneicosa-4,9,14,16,18,20-hexaene-4,9,14-tricarboxamide, 2,7,12-triphenyl-
(preparation of)

IT 61-54-1, Indole, 3-(2-aminoethyl)-
(reaction with glutaric acid derivs.)

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L20 ANSWER 1 OF 1 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA59:9970a CAOLD
TI action of base on quaternary salts of nicotinamide
AU Dittmer, Donald C.; Kolyer, J. M.
IT 952-92-1 1652-58-0 1893-57-8 2996-08-9 4533-64-6 5096-13-9
6621-73-4 6951-52-6 13502-54-0 19355-18-1 **63828-55-7**
75340-29-3 92578-90-0 93807-08-0 93897-69-9 93946-35-1 94379-06-3
95592-93-1 95592-94-2 95945-13-4 96003-72-4 96635-71-1 96650-48-5
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